

# Combustion Emissions from Refining Lower Quality Oil: What Is the Global Warming Potential?

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The greenhouse gas emission intensity of refining lower quality petroleum was estimated from fuel combustion for energy used by operating plants to process crude oils of varying quality. Refinery crude feed, processing, yield, and fuel data from four regions accounting for 97% of U.S. refining capacity from 1999 to 2008 were compared among regions and years for effects on processing and energy consumption predicted by the processing characteristics of heavier, higher sulfur oils. Crude feed density and sulfur content could predict 94% of processing intensity, 90% of energy intensity, and 85% of carbon dioxide emission intensity differences among regions and years and drove a 39% increase in emissions across regions and years. Fuel combustion energy for processing increased by approximately 61 MJ/m<sup>3</sup> crude feed for each 1 kg/m<sup>3</sup> sulfur and 44 MJ/m<sup>3</sup> for each 1 kg/m<sup>3</sup> density of crude refined. Differences in products, capacity utilized, and fuels burned were not confounding factors. Fuel combustion increments observed predict that a switch to heavy oil and tar sands could double or triple refinery emissions and add 1.6–3.7 gigatons of carbon dioxide to the atmosphere annually from fuel combustion to process the oil.

## Introduction

Replacing limited conventional crude oil (1) with heavy oil and natural bitumen (tar sands) resources could have substantial energy and environmental costs (2). Physical and chemical properties of the lower quality, heavier, more contaminated oils predict the combustion of more fuel for the energy necessary to convert them into product slates dominated by light hydrocarbon liquids (3–8). Preliminary estimates from fuel cycle analyses suggest that a switch to heavy oil and tar sands could increase the greenhouse gas emission intensity of petroleum energy by as much as 17–40%, with oil extraction and processing rather than tailpipe emissions accounting for the increment (3, 4). This raises the possibility that a switch to these oils might impede or foreclose the total reduction in emissions from all sources that is needed to avoid severe climate disruption. Accurate prediction of emissions from substitutes for conventional petroleum is therefore critical for climate protection. However, estimates of the emissions from processing lower quality oils have not been verified by observations from operating refineries.

Crude oils are extremely complex, widely ranging mixtures of hydrocarbons and organic compounds of heteroatoms

and metals (2, 7). Refiners use many distinct yet interconnected processes to separate crude into multiple streams, convert the heavier streams into lighter products, remove contaminants, improve product quality, and make multiple different products in varying amounts from crude of varying quality (5–11). Factors that affect emissions from refinery process energy consumption include crude feed quality, product slates, process capacity utilization, fuels burned for process energy, and, in some cases, preprocessing of refinery feeds near oil extraction sites. Estimates that construct process-by-process allocations of emissions among these factors have not been verified by observations from operating refineries in part because publicly reported data are limited for refinery-specific crude feeds and unavailable for process-level material and energy inputs and outputs (4–6). Research reported here distinguishes effects of crude feed quality on processing from those of the other factors using refinery-level data from multiple operating plants to estimate and predict the process energy consumption and resultant fuel combustion emissions from refining lower quality oil.

## Experimental Section

Refinery crude feed volume, density, and sulfur content, process capacity, capacity utilization, yield, and fuels were reported annually for each U.S. Petroleum Administration Defense District from 1999 to 2008 (9, 10). See the Supporting Information for this data (Table S1, Supporting Information). Districts 1 (East Coast-Appalachia), 2 (Midwest), 3 (Gulf Coast and vicinity), and 5 (West Coast, AK, and HI) each refined diverse crude feeds (19–41 source countries) at multiple facilities. Smaller, landlocked District 4 (Rocky Mountain states) refined nondiverse crude feeds (2–3 source countries).

At concentrations 4–8 times those of nitrogen and 160–500 times those of nickel and vanadium, sulfur is the major process catalyst poison in crude by mass (2, 11). In addition, for diverse blends of whole crude oils from many locations and geologic formations, distillation yield, and asphaltic, nitrogen, nickel, and vanadium content are roughly correlated with density and sulfur (2, 7). Variability in the effects of unreported crude feed characteristics on processing is thus constrained by the density and sulfur content of well-mixed crude feeds. Mixing analysis suggested that density and sulfur are reasonably reliable predictors of natural variability in unreported characteristics for annual crude feeds processed in Districts 1, 2, 3 and 5 but could not exclude the potential for unpredicted effects in processing the poorly mixed District 4 feed (Table S2, Supporting Information). The District 4 feed also was proportionately higher in synthetic crude oil (SCO) than those of other districts (Table S3, Supporting Information), and variant hydrogen production that was not predicted by crude feed density was found in District 4 (Table S4, Supporting Information). SCO may increase refinery hydroprocessing requirements (12, 13). High hydrogen capacity coincided with SCO refining in Districts 2 and 4 during 1999–2008, but the effect on refinery energy was minimal in District 2, while it was significant and more variable in District 4; other anomalies in the District 4 feed might cause this effect (Tables S2 and S4, Supporting Information). For these reasons, District 4 data were excluded from analysis of refinery observations and used only in estimates including upgrading for SCO. Districts 1, 2, 3, and 5 accounted collectively for 97% of U.S. refining capacity, 1999–2008. Analysis compared the reported data among these districts and years for interactions of the variables defined below.

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Oil quality (*OQ*) was defined as the density (*d*) and sulfur content (*S*) of crude feeds in mass per cubic meter (1 m<sup>3</sup>, 6.29 barrels oil; 264 gallons). The density of crude oils is proportional to the fraction of higher molecular weight, higher boiling point, larger hydrocarbon compounds in the oils that are distilled in a vacuum, then cleaved (cracked) into fuel-size compounds to make light hydrocarbon fuels. The larger hydrocarbons have lower hydrogen/carbon ratios that require hydrogen addition to improve product quality and higher concentrations of sulfur and other catalyst poisons that are freed by cracking and bonded with hydrogen to remove them from the oil and protect process catalysts (2, 11). This hydrocracking and hydrotreating of gas oil and residua uses several times more hydrogen than does hydrotreating of lighter streams such as naphtha (11). These processing characteristics require increased capacity for vacuum distillation, cracking, and hydroprocessing of gas oil and residua in refineries designed to make light liquid products from heavier, higher sulfur crude oils (4, 8, 14).

Crude processing intensity (*PI*) was thus defined as the ratio by volume of vacuum distillation capacity, conversion capacity (catalytic, thermal, and hydrocracking), and crude stream (gas oil and residua) hydrotreating capacity to atmospheric crude distillation capacity. These processes account for the primary processing acting on the crude and “reduced crude” that *Speight* distinguishes from secondary processes acting on product streams such as gasoline, naphtha, and distillate oils (7). *PI* measures the increasing portion of the crude input fed to these processes that is predicted by worsening *OQ* (increasing *d*, *S*, or both) and indicates the additional energy needed for heat, pressure, and reactants such as hydrogen to process those increasing feed volumes. It also defines an operational distinction between “crude stream” processing that acts on crude, gas oils, and residua and the subsequent “product stream” processing that acts on the unfinished products from crude stream processing. This distinction was useful in the absence of reported data for more detailed process-level analyses of material and energy flows. *PI* was analyzed with refinery-level crude feed, fuel, capacity utilization, and product yield data to verify the refinery process energy predicted by *OQ*.

Energy intensity (*EI*) was defined as total refinery process energy consumed per volume crude feed, based on reported fuels consumed (Table S1, Supporting Information). Purchased fuels consumed by refiners, such as electric power from the transmission grid, were included in *EI*. Energy used by hydrogen production plants was estimated based on 90% of production capacity and data for new natural gas-fed steam methane reforming facilities (10, 15, Table S1, Supporting Information). *EI* integrates all factors in refineries that consume fuel energy, allowing analysis of *EI* with *OQ* and processing to account for refinery capacity utilized and yield.

Effects of variable product slates on refinery energy consumption were distinguished from those of *OQ* in five ways. First, product slate effects on the relationships observed among crude feed quality, crude stream processing, and energy were estimated directly. This was done by including the products ratio, defined as the volume of gasoline, kerosene, distillate, and naphtha divided by that of other refinery products, as an explanatory variable in comparisons of *OQ*, *PI*, and *EI*. Second, the products ratio, combined yield of gasoline and distillate, and combined yield of petroleum coke and fuel gas were analyzed with *EI* and *OQ*. This quantified changes in refinery energy with yield and changes in yield with crude feed quality for key conversion products and byproducts. Third, energy use was analyzed with product stream process capacities to estimate changes in *EI* that could be explained by changes in product processing rates. Fourth, effects of product stream processing on energy for hydrogen were compared with those of crude stream processing by

analyzing hydrogen production capacity with product hydrotreating capacity, hydrocracking capacity, and *OQ*. Finally, estimated total energy for processing product slates (Eproducts) was analyzed with *OQ*. Eproducts was estimated based on product-specific factors developed by Wang et al. (6) and yield data (Tables S1 and S5, Supporting Information). Refinery capacity utilization was included as an explanatory variable in all comparisons.

Analysis was by partial least squares regression (PLS, XLSTAT 2009). PLS was used based on the expectation that explanatory (*x*) variables may be correlated, the primary interest in prediction of *y* (e.g., *EI*) and a secondary interest in the weights of *x* variables (e.g., *S* and *d*) in predicting *y*. Distributions of PLS residuals appeared normal (Shapiro-Wilk; Anderson-Darling; Lilliefors; Jarque-Bera tests,  $\alpha$  0.05).

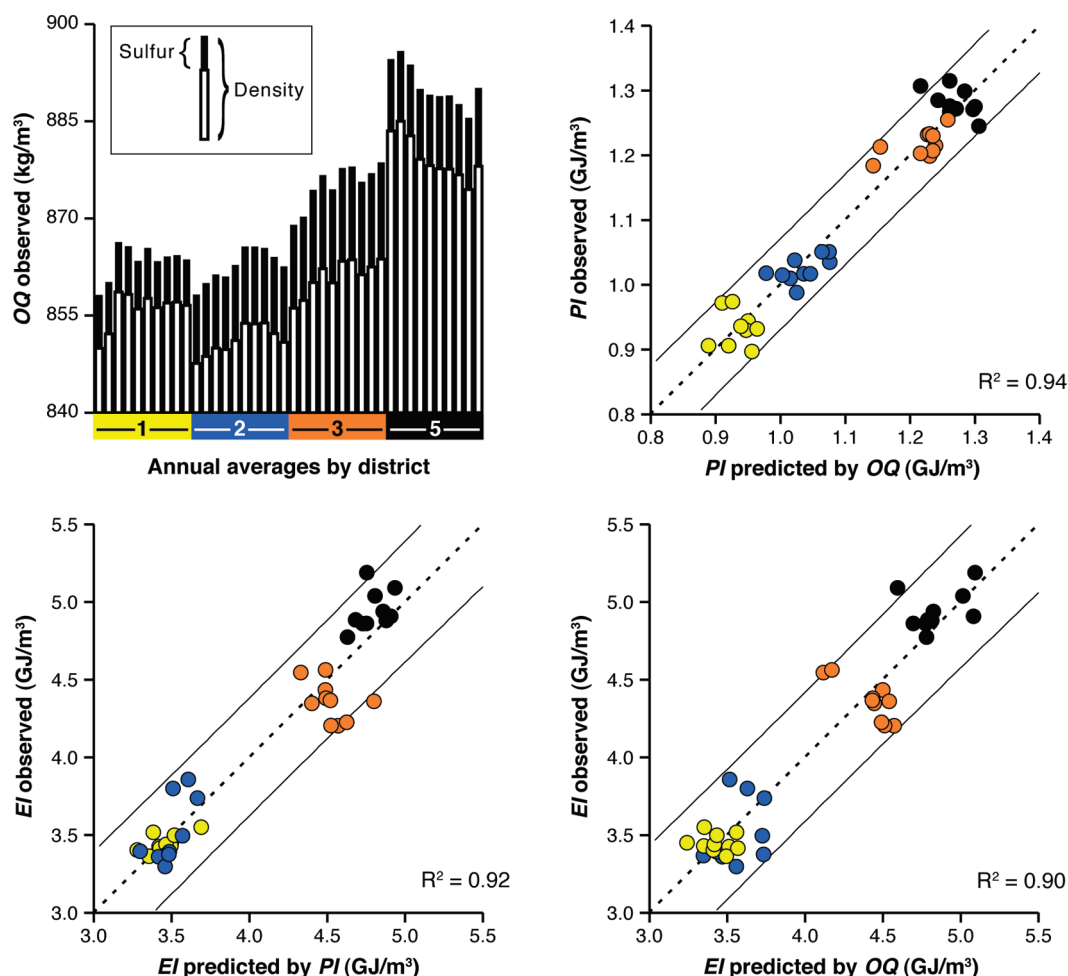
**Synthetic Crude Oil (SCO).** Coking- and hydrocracking-based upgrading of bitumen in Western Canada uses energy to yield SCO that has poor gas oil and distillate qualities but lower density and sulfur than the bitumen (12, 13). Refinery crude feeds and energy consumption do not reflect the original bitumen quality for this SCO or the energy used in its upgrading. SCO comprised appreciable fractions of annual crude feeds in Districts 2 (2–8%) and 4 (2–12%), based on limited estimates that may exclude SCO in some blended oil streams (Table S3, Supporting Information). Process modeling data for energy consumed and density and sulfur lost in coking- and hydrocracking-based upgrading (16) were applied to the estimated SCO volume in refinery feeds (Table S3, Supporting Information). Districts and years were compared for total processing (upgrading and refining) energy estimated and that predicted by including estimated original oil quality (*d*, *S*) in the prediction mode of the PLS model based on refinery observations (Table S6, Supporting Information).

**Emissions.** Emissions were assessed for carbon dioxide (CO<sub>2</sub>), the predominant greenhouse gas emitted by refineries (Table S7, Supporting Information). Direct measurements for all emission vents were not reported. Observed fuel consumption and fuel-specific emission factors developed by the U.S. Energy Information Administration (17, 18) were used to estimate “observed” emissions, and estimation details were documented (Table S1, Supporting Information). Fuel energy consumed ranged more widely among districts and years than the emission intensity of the fuel mix. Emissions predicted by *OQ* were based on *EI* predicted by *OQ* results from PLS and the emission intensity of the fuel mix. Observed and predicted emissions were compared among districts and years by PLS. Emissions estimates by government agencies (5, 19–21) that could be matched to data for *OQ* were superimposed on this comparison by including their *OQ* and predicted *EI* values in the prediction mode of the PLS models for the districts data (Tables S8 and S9, Supporting Information).

For heavy oil and natural bitumen, *OQ* data reported by the U.S. Geological Survey (2) and the average (1999–2008) U.S. refinery capacity utilization and products ratio were used in the prediction mode of the PLS model for observed *EI* versus *OQ* to predict *EI* (Table S8, Supporting Information). Predicted emissions from heavy oil and natural bitumen were derived from the products of these *EI* predictions (95% confidence for observations) and the emission intensity of the average (1999–2008) U.S. refinery fuel mix.

## Results

Figure 1 shows results from comparisons of *OQ*, *PI*, and *EI* among districts and years from 1999 to 2008. Observed *OQ* ranges by 7.85 kg/m<sup>3</sup> crude feed (kg/m<sup>3</sup>) for *S* and 37.6 kg/m<sup>3</sup> for *d*. Observed *PI* ranges by 0.42, or 42% of atmospheric crude distillation capacity. Observed *EI* ranges by 1.89 GJ/m<sup>3</sup> crude feed. *PI* is strongly and positively associated with



**FIGURE 1.** Increasing crude processing intensity and energy intensity with worsening oil quality. *OQ*: Crude feed oil quality. *PI*: Crude processing intensity. *EI*: Refinery energy intensity. Observations are annual weighted averages for districts 1 (yellow), 2 (blue), 3 (orange), and 5 (black) in 1999–2008. Diagonal lines bound the 95% confidence of prediction for observations.

worsening *OQ* (increasing *d*, *S*, or both). *EI* is strongly and positively associated with worsening *OQ* and increasing *PI*. *EI* increases by approximately 44 MJ/m<sup>3</sup> for each 1 kg/m<sup>3</sup> *d* and 61 MJ/m<sup>3</sup> for each 1 kg/m<sup>3</sup> *S* based on the PLS regression analysis for *EI* versus *OQ*. The equation of the model (*EI* vs *OQ*) can be expressed as

$$EI = 0.044d + 0.061S + 0.010(\text{Capacity utilized}) - 0.159(\text{Products ratio}) - 35.092 \quad (1)$$

where *EI* is the central prediction in GJ/m<sup>3</sup>, *d* is in kg/m<sup>3</sup>, *S* is in kg/m<sup>3</sup>, capacity utilized is in percent, products ratio is expressed as a quotient, and the last term is the coefficient for the intercept.

Table 1 shows additional results from analysis of refinery observations. *PI* increases strongly with *d* and *S* (95% confidence for observations). *EI* increases strongly with *d* and *S* and with vacuum distillation, conversion, and crude stream hydrotreating capacities. Hydrogen production capacity increases strongly with *d* and hydrocracking capacity. Sulfur recovery capacity increases strongly with *S*. These observations describe increasing portions of crude feeds processed by crude stream capacity and resultant effects on total refinery energy consumption as crude density and sulfur content increase.

In contrast to crude stream processing, except for cracking byproducts and two processes that treat them, product slate indicators are not significant or decrease with increasing *OQ* and *EI*. The products ratio is not significant in the strong relationships among *EI*, *PI*, and *OQ*, perhaps in part because

light liquids yield is less variable than *S* or *EI* among these districts and years. However, the ratio of light liquids to other products decreases with increasing *d* (products ratio vs *OQ*) and *EI* (*EI* vs products processing), and yield shifts, from gasoline and distillate to coke and fuel gas, as *OQ* worsens and *EI* increases.

Products processing reflects this shift from light liquids to cracking byproducts. Product stream hydrotreating, reforming, asphalt, aromatics, and polymerization/dimerization capacities decrease as *EI* increases. Those five processes account for 83–90% of total product stream processing capacity among districts (Table S1, Supporting Information). Among products processes, only alkylation and isomerization (7–13% of products capacity), which receive light streams from conversion processes, are positively associated with *EI*. Product hydrotreating cannot explain the observed increase in hydrogen production with increasing *d*. Estimated refinery energy use for products processing (*Eproducts*) decreases with increasing *d*. These results appear to measure the decreasing fraction of crude inputs converted to light liquid product streams and increasing creation of cracking byproducts such as coke and fuel gas that result from incomplete conversion as crude feed density and sulfur increase.

A weak inverse association of hydrogen production with product hydrotreating capacity (Table 1) results from a strong increase in H<sub>2</sub> capacity with *d* and hydrocracking, a steady decrease in the hydrotreating/hydrocracking ratio with increasing H<sub>2</sub> capacity, and lower hydrotreating at high



**TABLE 1. Results from Refinery Crude Feed Quality, Processing, Energy, Yield, and Emission Comparisons<sup>a</sup>**

effects of crude feed oil quality (OQ)					
y vs x	R <sup>2</sup>	standardized coefficients of x variables (coeff)			
		density	sulfur	cap. utilized	products ratio
process intensity (PI) vs OQ	0.94	<b>0.73</b>	<b>0.42</b>	<b>0.09</b>	−0.02
energy intensity (EI) vs OQ	0.90	<b>0.80</b>	<b>0.23</b>	0.05	−0.10
hydrogen production vs OQ	0.91	<b>1.09</b>	−0.01	0.05	<b>0.35</b>
sulfur recovery vs OQ	0.94	−0.01	<b>0.95</b>	−0.06	<b>−0.15</b>
pet. coke + fuel gas vs OQ	0.95	<b>0.80</b>	<b>0.34</b>	−0.04	
gasoline + distillate vs OQ	0.75	<b>−0.85</b>	−0.07	−0.04	
products ratio vs OQ	0.26	<b>−0.40</b>	−0.12	0.17	
Eproducts vs OQ	0.74	<b>−0.61</b>	0.13	<b>0.49</b>	

effects of oil quality (OQ) and fuels on CO <sub>2</sub> emissions			
y vs x	R <sup>2</sup>	standardized coefficients of x variables (coeff)	
		EI predicted by OQ	fuel mix emission intensity
observed vs predicted CO <sub>2</sub>	0.85	<b>0.88</b>	−0.04

effects of processing and products yield					
y vs x	R <sup>2</sup>	coeff.	y vs x	R <sup>2</sup>	coeff.
EI vs PI	0.92		EI vs yield	0.93	
vacuum distillation		<b>0.35</b>	pet. coke + fuel gas		<b>0.59</b>
conversion capacity		<b>0.35</b>	gasoline + distillate		<b>−0.42</b>
csHydrotreating		<b>0.22</b>	capacity utilized		−0.01
capacity utilized		<b>−0.16</b>	products ratio		−0.02
products ratio		−0.14			
H <sub>2</sub> production vs hydrocracking	0.97		EI vs psProcessing	0.91	
hydrocracking		<b>1.02</b>	psHydrotreating		<b>−0.17</b>
capacity utilized		−0.06	reforming		<b>−0.19</b>
products ratio		<b>0.14</b>	asphalt		<b>−0.30</b>
			aromatics		<b>−0.33</b>
H <sub>2</sub> production vs product-stream hydrotreating			polym./dimerization		<b>−0.25</b>
			lubricants		0.04
psHydrotreating	0.18	<b>−0.33</b>	alkylation		<b>0.30</b>
capacity utilized		−0.09	isomerization		<b>0.24</b>
products ratio		<b>−0.17</b>	capacity utilized		−0.06
			products ratio		<b>−0.33</b>

<sup>a</sup> R-squared values and standardized coefficients from PLS regressions on annual data from refining districts 1, 2, 3 and 5, 1999–2008. **Boldface:** significant at 95% confidence. Eproducts: estimated energy use to process a given product slate. Prefix cs (ps): crude stream (product stream) processing.

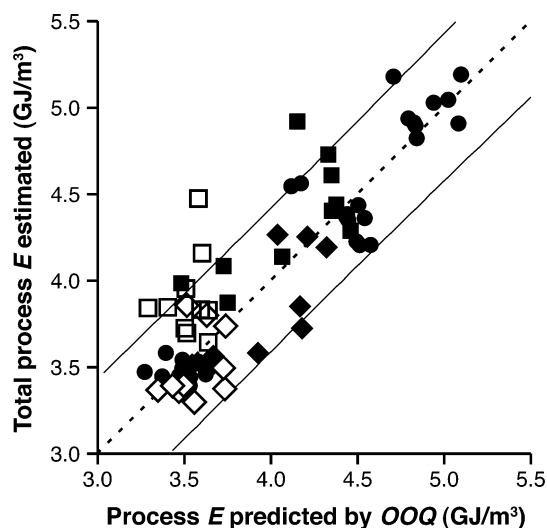
H<sub>2</sub> capacity among these districts and years (Figure S1, Supporting Information). Refinery capacity utilization was not significant in the effects of OQ on EI and affected the relationships between PI and OQ and between PI and EI only marginally, possibly because capacity utilization varied little among districts and years (Table S1, Supporting Information). Significant capacity utilization results are consistent with marginally increased energy consumption and decreased flexibility to process lower quality crude when refineries run closer to full capacity.

Rough estimates including the energy, *d*, and *S* lost in bitumen upgrading for SCO refined reveal greater effects of total processing for crude feeds refined in Districts 2 and 4 and follow the relationships observed in refining (Figure 2). Estimated total processing energy falls within the prediction based on OQ from refinery observations in 43 of 50 cases and exceeds the 95% confidence of prediction by more than 2% only in two cases explained by District 4 hydrogen anomalies discussed above. Oil quality–energy relationships observed in refining can predict those for total processing because upgrading and refining use similar carbon rejection, hydrogen addition, and utility technology.

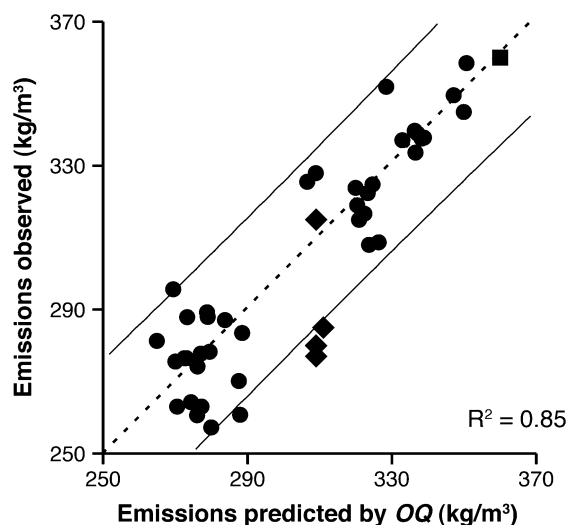
Emissions calculated from observed fuels consumed are strongly and positively associated with EI predicted by OQ (Table 1) and range by 39%, from 257 to 358 kg/m<sup>3</sup> crude

feed (Figure 3). Observed emissions fall within the 95% confidence of prediction based on OQ in 36 of 40 cases and are within 3% of the confidence of prediction in all cases. Despite emission differences among fuels, the fuel mix is not significant in this prediction. The emission intensity of the fuel mix varies much less than EI and decreases slightly with decreasing petroleum coke contributions and a shift in cracking processes as EI, *d*, and *S* increase (Table S1 and Figure S1, Supporting Information). Refinery emission estimates by government agencies that could be matched to OQ differ from each other by as much as 12–30% but fall within 2% of the central prediction based on OQ or within 4% of its confidence interval (5, 19–21, Table S8, Supporting Information). The 2008 San Francisco Bay Area estimate in Figure 3 (360 kg/m<sup>3</sup>) is close to estimated 2008 California refinery emissions (354 kg/m<sup>3</sup>) (21), for which matching OQ data were not available. California gasoline and diesel production may account for 56% (197.2 kg) and 22% (78.7 kg) of this 354 kg/m<sup>3</sup>, respectively, based on fuel-specific estimates for the average California crude feed (21–23, Table S8, Supporting Information).

Predictions for heavy oil (957.4 kg/m<sup>3</sup> *d*; 27.8 kg/m<sup>3</sup> *S*) and natural bitumen (1 033.6 kg/m<sup>3</sup> *d*; 45.5 kg/m<sup>3</sup> *S*) (USGS average) (2) reflect their low quality compared with crude feeds observed (Figure 1). On the basis of the PLS model for



**FIGURE 2.** Estimated process energy for bitumen upgrading and refining versus that predicted by oil quality (GJ/m<sup>3</sup> crude), 1999–2008. *OQ*: original oil quality including bitumen quality for synthetic oil inputs. Black diamonds: District 2. Black squares: District 4. Black circles: Districts 1, 3, and 5. White diamonds (squares): District 2 (District 4) refinery energy and oil quality only. Diagonal lines bound the 95% confidence of prediction for refinery observations.



**FIGURE 3.** Refinery CO<sub>2</sub> emission intensity observed versus predicted by oil quality. *OQ*: Oil quality. Black circles: District 1, 2, 3, or 5 annually, 1999–2008. Black diamonds: United States in 2002, 2005, 2006, 2007. Black square: San Francisco Bay Area in 2008. Diagonal lines bound the 95% confidence of prediction for observations.  $R^2$  value shown is for the comparison among districts and years.

observations from Districts 1, 2, 3, and 5 (*EI* vs *OQ*) and the emission intensity of the U.S. refinery fuel mix (73.8 kg/GJ), processing the range of heavy oil/bitumen blends could use 8.23–14.13 GJ/m<sup>3</sup> fuel (Table S8, Supporting Information) and emit 0.61–1.04 t/m<sup>3</sup> CO<sub>2</sub>.

## Discussion

Strongly coupled increases in energy and crude stream processing intensities with worsening oil quality (Figure 1) describe energy for carbon rejection, aggressive hydrogen addition, and supporting processes acting on larger portions of heavier, higher sulfur crude feeds to yield light liquid product streams. The creation of cracking reaction byproducts that limits conversion of heavier oils to light liquid

product streams is observed in the shift from gasoline and distillate to coke and fuel gas yield as *OQ* worsens and *EI* increases. Observed decreases in light liquids yield and most major product stream processes as *EI* increases are consistent with this rising reliance on incomplete conversion. Differences in product slates cannot explain increasing *EI* as *OQ* worsens because capacities of processes comprising 83–90% of product stream processing capacity decrease as *EI* increases, and estimated energy use for products processing decreases as *OQ* worsens. Hydrogen production increases with crude density and hydrocracking. *EI* drives emissions variability. *OQ* predicts 94% of *PI*, *PI* predicts 92% of *EI*, and *OQ* predicts 90% of *EI* and 85% of emissions variability. These observations from operating plants across the four largest U.S. refining districts over 10 years provide evidence that crude feed density and sulfur content predict processing, energy, and CO<sub>2</sub> emission intensities for large groups of refineries with diverse feeds.

Slight, unexpected decreases in product hydrotreating at high hydrogen production and in fuel mix emission intensity with increasing *d* and *S* can be explained by a coincident shift from hydrotreating and catalytic cracking to hydrocracking with worsening *OQ*. Refiners can substitute hydrocracking for hydrotreating and catalytic cracking to some extent. *OQ*, along with other factors beyond this study scope, may influence those business decisions.

Energy increments predicted by density (44 MJ/kg) and sulfur (61 MJ/kg) in crude feeds (eq 1) compare to energy inputs of 40–70 MJ/kg density (including sulfur) lost from bitumen upgrading for SCO, based on process modeling of coking- and hydrocracking-based upgraders ((16), Table S6, Supporting Information). At an energy cost of 16.4 MJ/m<sup>3</sup> (Table S1, Supporting Information), hydrogen for density reduction by hydrocracking could account for 44 MJ/kg, based on the H<sub>2</sub>/oil feed ratio of 308 m<sup>3</sup>/m<sup>3</sup> Robinson and Dolbear report for 22°API feed and 44°API yield (11).

Results help to explain differences among government estimates of refinery emissions (Figure 3) and support the high case fuel cycle emission increments from a switch to heavy and tar sands oils reported for gasoline by Brandt and Farrel (+40%) (3) and for diesel by Gerdes and Skone (+17%) (4). Predicted emissions from processing heavy oil/natural bitumen blends (0.61–1.04 t/m<sup>3</sup>) are 2–3 times the average of observed and estimated emissions in Figure 3 (0.30 t/m<sup>3</sup>). Assuming this 0.30 t/m<sup>3</sup> refining average and 2007 world petroleum emissions (11.27 Gt) (24) as a baseline, processing heavy oil/bitumen blends at 2009 world refining capacity ( $5.06 \times 10^9$  m<sup>3</sup>) (10) could increase annual CO<sub>2</sub> emissions by 1.6–3.7 gigatons and total petroleum fuel cycle emissions by 14–33%. Extraction emissions would add to these percentages.

This prediction applies to average CO<sub>2</sub> emissions from large, multiplant refinery groups with diverse, well-mixed crude feeds and appears robust for that application. However, the method used here should be validated for other applications. If it is applied to different circumstances, the potential for significantly different product slates, poorly mixed crude feeds, synthetic crude oil impacts on refining, and effects on fuel mix emission intensity and hydrotreating resulting from choices among carbon rejection and hydrogen addition technologies should be examined.

Several issues suggest future work. Other properties of crude feeds and incremental efficiencies from modernization of equipment and catalyst systems might explain up to 10% of the variability in *EI* observed among U.S. refining districts and years and could be more important for single plants and nondiverse crude feeds. Burning more fuel to refine lower quality oil emits toxic and ozone-precursor combustion products along with CO<sub>2</sub>. Pastor et al. estimate that refinery emissions of such “co-pollutants” dominate health risk in nearby communities associated with particulate matter

emitted by the largest industrial sources of greenhouse gases in California and identify racial disparities in this risk as important in emission assessment (25). Better facility-level OQ data could improve local-scale pollutant assessment. Better crude quality predictions could improve energy, and climate protection, forecasts. Assessments of the need, scope, and timing for transition to sustainable energy should account for emissions from lower quality oil.

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## Supporting Information Available

Data and details of methods, analyses, and results. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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**Supporting information for the manuscript:**

**Combustion emissions from refining lower quality oil: What is the global warming potential?**

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Supporting information given in the following 49 pages includes tables S1–S9, Figure S1, and references. Each table includes a legend and notes narrative that follows the values given, as does the figure. References identify sources of data cited. This information appears as follows:

Pages S2-14:	<b>Table S1.</b> Data.
Pages S15-19:	<b>Table S2.</b> Simplified mixing analysis for potential effects of anomalous oils on crude feeds.
Pages S20-23:	<b>Table S3.</b> Estimate calculation for Canadian synthetic crude oil (SCO) exports to districts and years.
Pages S24-26:	<b>Table S4.</b> Evidence for effects of synthetic oil (SCO) on refinery processing during 1999-2008 in District 4.
Page S27:	<b>Table S5.</b> Efficiency factors for processing refinery products.
Pages S28-34:	<b>Table S6.</b> Estimate calculation, oil quality and processing <i>EI</i> including bitumen upgrading.
Page S35:	<b>Table S7.</b> Contribution of CO <sub>2</sub> to CO <sub>2</sub> e emitted by oil refineries.
Pages S36-40:	<b>Table S8.</b> PLS inputs for emissions predicted by <i>OQ</i> , and comparison emission estimates.
Page S41:	<b>Table S9.</b> Estimate calculation, San Francisco Bay Area crude feed <i>OQ</i> in 2008.
Pages S42-43:	<b>Figure S1.</b> Some shifts among hydrogen addition and carbon rejection technologies affecting relationships between (A) hydrotreating and hydrogen production, and (B) fuel mix emission intensity and crude feed density, across districts 1, 2, 3 and 5, 1999-2008.
Pages S44-49:	<b>References.</b>

# Supporting Information

**Table S1**

US		Refinery crude inputs <sup>a</sup> -----				Refinery process capacity <sup>b</sup> --			
District	Year	Feed volume	Density	Sulfur	Source	Atm. dist.	Vacuum dist.	Coking & therm.	Cat. cracking
PADD		(m <sup>3</sup> /d•10 <sup>4</sup> )	(kg/m <sup>3</sup> )	(kg/m <sup>3</sup> )	countries	(m <sup>3</sup> /d•10 <sup>4</sup> )	(m <sup>3</sup> /d•10 <sup>4</sup> )	(m <sup>3</sup> /d•10 <sup>4</sup> )	(m <sup>3</sup> /d•10 <sup>4</sup> )
1	1999	24.436	858.199	8.239	24	24.365	9.802	1.420	10.476
1	2000	24.754	860.182	8.000	23	24.592	9.721	1.440	10.798
1	2001	23.546	866.344	7.710	19	24.958	9.658	1.409	9.924
1	2002	24.246	865.708	7.445	20	25.222	9.742	1.442	9.899
1	2003	25.184	863.436	7.426	21	25.075	9.975	1.448	9.827
1	2004	24.961	865.443	7.789	21	25.025	9.974	1.448	9.827
1	2005	25.422	863.384	7.166	22	25.263	10.150	1.448	9.970
1	2006	23.626	864.122	7.172	21	25.263	10.149	1.448	9.970
1	2007	23.419	864.333	7.260	24	25.263	10.149	1.448	9.970
1	2008	22.115	863.647	7.082	24	25.263	10.149	1.448	9.970
2	1999	53.626	858.252	10.642	15	57.095	23.272	5.880	19.325
2	2000	54.215	860.025	11.352	16	56.984	23.625	6.098	19.189
2	2001	52.609	861.334	11.370	15	56.427	22.989	6.131	18.822
2	2002	51.162	861.019	11.279	20	55.775	22.592	5.698	18.688
2	2003	51.258	862.804	11.648	16	55.587	22.669	5.612	18.475
2	2004	52.482	865.655	11.859	20	55.528	22.961	5.818	18.268
2	2005	52.688	865.655	11.946	23	56.465	23.689	5.962	18.555
2	2006	52.609	865.443	11.597	20	56.506	23.895	5.948	18.538
2	2007	51.480	864.069	11.838	17	57.873	23.169	6.032	18.010
2	2008	51.575	862.594	11.731	16	57.980	23.466	5.923	18.676
3	1999	111.689	869.004	12.861	33	123.434	57.573	15.493	43.165
3	2000	113.024	870.287	12.967	31	123.436	59.107	16.498	43.434
3	2001	115.600	874.428	14.341	28	123.625	58.157	17.318	44.964
3	2002	112.786	876.703	14.466	33	125.817	57.449	18.717	46.010
3	2003	116.013	874.482	14.429	30	126.876	58.417	19.390	45.821
3	2004	119.145	877.791	14.396	33	128.032	60.442	20.047	46.126
3	2005	114.534	878.009	14.399	36	132.323	59.682	19.897	46.475
3	2006	117.253	875.673	14.361	41	133.383	59.850	20.190	46.632
3	2007	117.682	876.975	14.470	37	134.189	61.054	20.938	46.728
3	2008	111.879	878.663	14.937	36	133.771	61.411	21.046	47.311
5	1999	41.973	894.607	11.093	24	49.484	23.172	9.594	12.630
5	2000	43.086	895.853	10.840	23	49.836	23.152	9.714	12.717
5	2001	44.262	893.759	10.993	26	49.542	23.692	9.757	12.695
5	2002	44.787	889.993	10.858	27	48.422	23.419	9.834	12.768
5	2003	45.661	889.098	10.936	29	48.924	23.597	9.671	12.604
5	2004	45.486	888.874	11.200	28	48.723	23.478	9.695	12.717
5	2005	46.090	888.986	11.379	27	49.104	23.538	9.735	12.762
5	2006	45.693	887.648	10.918	30	49.441	23.930	9.759	13.026
5	2007	44.373	885.537	11.069	30	49.609	24.031	10.003	13.332
5	2008	44.739	890.161	12.106	30	49.730	24.411	9.793	13.170
4	1999	8.029	854.468	11.706	3	8.603	3.464	0.663	2.826
4	2000	8.156	859.346	12.031	2	8.094	3.130	0.663	2.705
4	2001	8.077	859.190	11.084	2	8.802	3.549	0.663	2.768
4	2002	8.363	860.234	12.043	2	9.054	3.616	0.676	2.898
4	2003	8.442	861.229	12.488	2	9.019	3.596	0.687	2.906
4	2004	8.856	862.594	11.645	2	9.296	4.255	0.695	2.950
4	2005	8.935	862.910	11.218	2	9.129	3.502	0.711	2.920
4	2006	8.856	860.496	11.359	2	10.018	3.560	0.711	3.121
4	2007	8.681	862.384	11.728	2	10.016	3.472	0.727	3.151
4	2008	8.585	863.120	12.170	2	9.555	3.305	0.989	2.832
US	1999	239.753	869.111	11.559	--	262.981	117.283	33.050	88.422
US	2000	243.235	870.822	11.669	--	262.942	118.735	34.413	88.844
US	2001	244.077	873.510	12.404	--	263.354	118.046	35.278	89.173
US	2002	241.343	873.888	12.322	--	264.289	116.819	36.368	90.263
US	2003	246.558	872.864	12.482	--	265.481	118.253	36.809	89.633
US	2004	250.930	875.185	12.515	--	266.604	121.109	37.703	89.887
US	2005	247.670	875.077	12.426	--	272.284	120.561	37.753	90.682
US	2006	248.052	873.780	12.320	--	274.612	121.385	38.056	91.286
US	2007	245.635	873.888	12.497	--	277.389	124.553	39.148	91.191
US	2008	238.910	875.023	12.863	--	276.299	122.742	39.198	91.959
Energy factor <sup>c</sup>		--	--	--	--	--	--	--	--
CO <sub>2</sub> emission		--	--	--	--	--	--	--	--
factor (kg/GJ) <sup>c</sup>		--	--	--	--	--	--	--	--



# Supporting Information

**Table S1 continued**

US Refinery process capacity <sup>b</sup> ----									
District	Year	Hydrocracking	csHydrotreating	psHydrotreating	Reforming	Alkylation	Pol./Dim.	Aromatics	Isomerization
PADD		(m <sup>3</sup> /d•10 <sup>4</sup> )	(m <sup>3</sup> /d•10 <sup>4</sup> )	(m <sup>3</sup> /d•10 <sup>4</sup> )	(m <sup>3</sup> /d•10 <sup>4</sup> )	(m <sup>3</sup> /d•10 <sup>4</sup> )	(m <sup>3</sup> /d•10 <sup>4</sup> )	(m <sup>3</sup> /d•10 <sup>4</sup> )	(m <sup>3</sup> /d•10 <sup>4</sup> )
1	1999	0.666	1.320	12.826	4.567	1.282	0.284	0.861	0.447
1	2000	0.666	1.320	12.460	4.468	1.346	0.284	0.852	0.431
1	2001	0.680	0.715	13.030	4.483	1.281	0.212	0.852	0.526
1	2002	0.602	2.131	12.214	4.528	1.292	0.212	0.852	0.611
1	2003	0.602	1.473	13.779	4.548	1.290	0.212	0.852	0.868
1	2004	0.603	1.477	13.513	4.649	1.290	0.212	0.852	0.878
1	2005	0.603	1.477	13.227	4.681	1.335	0.212	0.852	0.878
1	2006	0.615	0.704	13.993	4.681	1.335	0.212	0.852	0.878
1	2007	0.615	0.704	14.057	4.681	1.335	0.212	0.852	0.878
1	2008	0.615	0.704	14.057	4.681	1.335	0.212	0.852	0.878
2	1999	2.533	7.126	29.912	13.533	3.927	0.208	0.924	2.796
2	2000	2.533	6.099	31.548	13.770	3.959	0.208	0.924	2.764
2	2001	2.386	5.401	32.961	13.435	3.940	0.208	0.924	2.757
2	2002	2.434	7.177	31.440	13.357	3.892	0.136	0.888	2.698
2	2003	2.410	7.355	34.844	13.339	3.835	0.136	0.888	2.863
2	2004	2.191	8.214	35.157	13.247	3.807	0.129	0.876	2.900
2	2005	2.798	8.330	38.089	13.368	3.984	0.128	0.838	2.908
2	2006	3.065	7.937	39.013	13.347	3.991	0.128	0.919	2.940
2	2007	3.701	7.929	38.528	13.460	3.911	0.128	0.657	2.944
2	2008	3.652	8.440	36.890	12.972	3.871	0.130	0.657	2.784
3	1999	11.265	18.638	64.038	27.308	8.602	0.310	4.081	4.523
3	2000	11.513	19.190	65.900	27.730	8.599	0.297	4.202	4.347
3	2001	11.842	15.900	70.483	26.840	8.514	0.297	4.260	4.291
3	2002	12.138	18.588	70.415	27.234	9.806	0.353	4.310	4.551
3	2003	11.359	21.356	76.385	27.088	8.982	0.355	4.072	4.572
3	2004	11.868	22.256	82.382	27.517	10.514	0.378	4.386	4.472
3	2005	11.439	22.191	87.486	26.859	9.144	0.347	4.354	4.345
3	2006	11.447	22.301	90.603	26.857	9.253	0.345	4.239	4.312
3	2007	12.059	24.717	91.006	27.458	8.907	0.646	5.026	3.923
3	2008	11.843	22.910	94.039	27.091	9.179	0.646	5.786	4.284
5	1999	8.089	9.630	21.588	8.763	2.928	0.224	0.040	2.097
5	2000	8.119	8.347	22.626	8.849	4.181	0.234	0.040	2.142
5	2001	8.192	8.614	22.642	8.950	2.933	0.234	0.045	2.142
5	2002	8.192	9.472	21.821	8.833	2.999	0.234	0.045	2.147
5	2003	8.043	8.053	23.957	8.847	3.114	0.235	0.045	2.716
5	2004	8.138	8.151	24.765	8.895	3.119	0.238	0.040	2.659
5	2005	8.259	8.154	24.643	8.946	3.153	0.250	0.036	2.727
5	2006	8.896	7.932	25.742	9.400	3.359	0.280	0.021	2.937
5	2007	9.221	8.274	26.024	9.634	3.362	0.228	0.019	3.258
5	2008	9.124	8.123	26.175	9.473	3.337	0.228	0.019	3.171
4	1999	0.079	0.965	4.702	1.901	0.578	0.073	0.000	0.245
4	2000	0.079	0.744	4.368	1.770	0.525	0.067	0.000	0.245
4	2001	0.278	0.437	5.062	1.905	0.586	0.083	0.000	0.236
4	2002	0.079	0.783	4.784	1.889	0.612	0.083	0.000	0.236
4	2003	0.087	0.783	5.090	1.901	0.622	0.083	0.000	0.238
4	2004	0.254	0.836	4.673	1.772	0.566	0.076	0.000	0.239
4	2005	0.087	0.852	5.123	1.917	0.583	0.097	0.000	0.239
4	2006	0.254	1.092	5.444	1.940	0.596	0.097	0.000	0.258
4	2007	0.280	1.092	5.607	1.953	0.604	0.097	0.000	0.264
4	2008	0.087	1.302	5.720	1.816	0.612	0.083	0.000	0.264
US	1999	22.632	37.678	133.066	56.072	17.317	1.099	5.906	10.108
US	2000	22.910	35.699	136.901	56.585	18.609	1.090	6.017	9.929
US	2001	23.379	31.067	144.178	55.613	17.254	1.034	6.080	9.952
US	2002	23.446	38.151	140.674	55.840	18.602	1.018	6.093	10.243
US	2003	22.502	39.021	154.054	55.723	17.842	1.020	5.856	11.258
US	2004	23.054	40.935	160.490	56.081	19.295	1.034	6.154	11.148
US	2005	23.186	41.005	168.568	55.771	18.200	1.033	6.079	11.097
US	2006	24.278	39.967	174.794	56.226	18.534	1.062	6.032	11.324
US	2007	25.876	42.717	175.222	57.186	18.119	1.311	6.554	11.268
US	2008	25.322	41.479	176.881	56.034	18.333	1.299	7.314	11.381
Energy factor <sup>c</sup>		--	--	--	--	--	--	--	--
CO <sub>2</sub> emission		--	--	--	--	--	--	--	--
factor (kg/GJ) <sup>c</sup>		--	--	--	--	--	--	--	--

# Supporting Information

**Table S1 continued**

US		Refinery process capacity <sup>b</sup> ---			Fuels consumed in refineries <sup>a</sup> -----				
District	Year	Lubes	Asphalt	Sulfur	H <sub>2</sub> production	Crude oil	LPG	Distillate	Res. fuel oil
PADD		(m <sup>3</sup> /d•10 <sup>4</sup> )	(m <sup>3</sup> /d•10 <sup>4</sup> )	(kg/d•10 <sup>6</sup> )	(m <sup>3</sup> •10 <sup>8</sup> )	(m <sup>3</sup> •10 <sup>4</sup> )	(m <sup>3</sup> •10 <sup>4</sup> )	(m <sup>3</sup> •10 <sup>4</sup> )	(m <sup>3</sup> •10 <sup>4</sup> )
1	1999	0.368	1.033	0.921	11.783	0.000	2.766	2.035	37.012
1	2000	0.300	0.461	0.921	14.056	0.000	5.008	4.165	38.904
1	2001	0.300	0.461	0.856	11.576	0.000	5.819	8.967	44.675
1	2002	0.299	0.445	1.265	10.232	0.000	4.483	7.631	29.190
1	2003	0.299	0.445	1.301	15.090	0.000	7.854	9.921	28.014
1	2004	0.300	0.445	1.301	15.090	0.000	7.870	7.409	18.013
1	2005	0.300	0.445	1.319	15.297	0.000	11.479	5.819	18.220
1	2006	0.300	0.445	1.319	17.364	0.000	5.231	0.366	14.627
1	2007	0.300	0.445	1.285	13.333	0.000	2.941	0.350	13.132
1	2008	0.300	0.445	1.285	13.333	0.000	0.827	0.461	6.344
2	1999	0.264	3.493	4.436	44.237	0.000	27.123	0.986	43.531
2	2000	0.264	3.763	4.402	44.030	0.000	14.484	0.763	34.166
2	2001	0.264	3.617	4.425	47.751	0.000	13.975	1.288	38.888
2	2002	0.277	3.668	4.672	43.926	0.000	16.439	1.081	29.747
2	2003	0.277	3.727	4.818	40.619	0.000	25.804	0.588	9.380
2	2004	0.277	3.705	4.631	41.032	0.000	17.155	0.588	3.100
2	2005	0.269	3.814	5.140	49.611	0.000	12.385	0.795	2.591
2	2006	0.269	3.897	5.243	77.000	0.000	9.015	0.715	3.275
2	2007	0.269	3.151	4.600	77.931	0.000	13.387	0.747	3.005
2	2008	0.135	3.608	5.200	78.551	0.000	12.783	0.700	3.084
3	1999	1.786	1.930	14.092	146.456	0.159	12.560	1.892	0.191
3	2000	1.801	1.967	15.297	148.833	0.000	13.085	2.798	0.032
3	2001	1.772	1.848	15.266	155.655	0.000	11.018	2.178	0.000
3	2002	1.745	1.904	16.516	160.512	0.000	13.450	1.335	0.000
3	2003	1.793	2.569	17.134	160.512	0.000	17.489	0.700	0.000
3	2004	1.982	2.409	19.395	174.362	0.000	5.898	1.304	0.000
3	2005	2.343	1.936	19.135	172.398	0.000	5.708	1.367	0.064
3	2006	2.351	1.914	19.393	162.269	0.000	4.404	1.765	0.016
3	2007	2.282	1.938	19.013	160.822	0.000	3.307	1.828	0.048
3	2008	2.281	1.938	19.243	164.233	0.000	8.204	1.701	0.048
5	1999	0.437	1.191	4.152	126.301	0.000	18.649	4.086	9.015
5	2000	0.437	1.215	4.152	151.934	0.000	34.150	3.736	11.081
5	2001	0.437	1.078	4.152	149.247	0.000	47.251	4.436	13.609
5	2002	0.342	0.742	4.230	151.004	0.000	19.587	3.307	14.341
5	2003	0.342	0.979	4.331	148.523	0.000	34.484	3.911	11.558
5	2004	0.286	0.920	4.286	147.903	0.000	24.627	3.657	11.495
5	2005	0.286	0.940	4.520	149.557	0.000	36.424	4.022	11.558
5	2006	0.318	0.916	4.911	159.169	0.000	23.339	4.054	12.242
5	2007	0.318	0.940	4.539	162.786	0.000	22.497	3.752	11.813
5	2008	0.318	0.940	5.011	162.786	0.000	23.991	4.642	11.845
4	1999	0.000	0.688	0.381	8.889	0.000	0.636	0.095	3.450
4	2000	0.000	0.671	0.382	8.992	0.000	0.890	0.048	4.786
4	2001	0.000	0.838	0.367	9.612	0.000	0.620	0.111	3.482
4	2002	0.000	0.738	0.368	9.612	0.000	0.700	0.000	3.259
4	2003	0.000	0.738	0.538	9.199	0.000	0.779	0.000	2.671
4	2004	0.000	0.743	0.612	9.509	0.000	1.065	0.016	2.337
4	2005	0.000	0.576	13.577	13.953	0.000	0.382	0.000	2.655
4	2006	0.000	0.796	0.593	13.953	0.000	0.238	0.000	1.924
4	2007	0.000	0.783	0.599	18.191	0.000	0.207	0.000	1.320
4	2008	0.000	0.807	0.595	20.878	0.000	0.779	0.000	0.779
US	1999	2.856	8.335	23.982	337.665	0.159	61.735	9.094	93.198
US	2000	2.803	8.077	25.154	367.845	0.000	67.617	11.511	88.969
US	2001	2.774	7.842	25.066	373.840	0.000	78.683	16.980	100.655
US	2002	2.662	7.498	27.051	375.287	0.000	54.660	13.355	76.536
US	2003	2.710	8.458	28.122	373.943	0.000	86.410	15.120	51.623
US	2004	2.845	8.222	30.225	387.896	0.000	56.615	12.973	34.945
US	2005	3.199	7.712	43.691	400.816	0.000	66.377	12.004	35.088
US	2006	3.239	7.967	31.459	429.756	0.000	42.227	6.900	32.084
US	2007	3.169	7.256	30.036	433.063	0.000	42.338	6.677	29.317
US	2008	3.035	7.737	31.334	439.781	0.000	46.583	7.504	22.099
Energy factor <sup>c</sup>		--	--	--	16.4 MJ/m <sup>3</sup>	38.49 GJ/m <sup>3</sup>	25.62 GJ/m <sup>3</sup>	38.66 GJ/m <sup>3</sup>	41.72 GJ/m <sup>3</sup>
CO <sub>2</sub> emission factor (kg/GJ) <sup>c</sup>		--	--	--	52.70	78.53	65.76	77.18	83.14

# Supporting Information

**Table S1 continued**

US Fuels consumed in refineries <sup>a</sup>								
District	Year	Fuel gas (bl)	Pet. coke	Other prod-	Natural gas	Coal	Electricity pur-	Steam pur-
PADD		(m <sup>3</sup> •10 <sup>5</sup> )	(m <sup>3</sup> •10 <sup>5</sup> )	uct (m <sup>3</sup> •10 <sup>4</sup> )	(m <sup>3</sup> •10 <sup>8</sup> )	(Gg)	chased (TWh)	chased (Tg)
1	1999	32.387	20.538	6.964	11.501	28.123	3.180	1.599
1	2000	31.990	19.093	6.105	12.553	27.216	3.084	1.897
1	2001	32.322	18.975	5.406	9.915	29.030	3.450	1.797
1	2002	33.987	18.805	5.851	11.086	28.123	3.282	1.865
1	2003	35.329	19.649	7.059	8.032	29.030	3.415	1.674
1	2004	35.419	20.377	2.242	9.177	26.308	3.410	2.352
1	2005	35.481	20.369	2.242	10.082	29.937	3.520	2.228
1	2006	33.756	17.541	0.859	10.258	28.123	3.576	2.593
1	2007	36.392	19.036	0.334	8.129	29.030	3.984	2.624
1	2008	33.909	19.393	0.461	7.892	28.123	4.192	2.360
2	1999	76.667	29.697	22.560	26.317	0.000	8.956	1.262
2	2000	77.341	29.335	19.047	30.038	1.814	8.949	0.890
2	2001	76.697	27.643	20.382	26.510	6.350	8.728	2.060
2	2002	73.293	27.689	19.555	27.235	0.000	8.933	2.368
2	2003	72.970	27.357	16.392	26.727	8.165	8.885	2.577
2	2004	79.249	25.339	27.855	29.254	7.257	9.486	2.863
2	2005	79.832	27.572	26.805	30.152	7.257	9.875	2.283
2	2006	78.834	26.236	31.177	32.485	2.722	10.488	3.310
2	2007	78.586	24.963	6.280	33.993	6.350	10.555	4.871
2	2008	77.716	23.856	0.286	39.330	10.886	10.804	4.999
3	1999	181.263	66.223	31.177	147.683	0.000	13.762	8.968
3	2000	184.163	67.454	34.405	147.541	0.000	14.501	11.455
3	2001	177.565	66.822	30.923	138.325	0.000	15.868	13.142
3	2002	181.193	66.891	21.479	129.876	0.000	16.145	14.670
3	2003	194.971	67.972	29.874	121.706	0.000	15.682	14.456
3	2004	190.864	69.595	22.544	111.896	0.000	17.044	14.827
3	2005	177.745	65.660	20.668	112.129	0.000	16.620	15.757
3	2006	198.807	72.481	31.336	112.029	0.000	18.612	17.690
3	2007	192.263	67.964	24.007	102.791	0.000	20.433	28.790
3	2008	181.956	62.598	26.996	107.893	0.000	20.675	28.919
5	1999	72.803	21.174	25.851	34.754	0.000	5.389	8.469
5	2000	74.282	22.314	26.185	38.268	0.000	4.809	8.268
5	2001	77.031	22.827	22.576	34.867	0.000	4.695	7.881
5	2002	70.694	22.640	22.672	38.733	0.000	4.780	7.589
5	2003	74.354	23.823	25.740	37.477	0.000	4.520	8.595
5	2004	73.964	24.441	31.305	35.335	0.000	4.871	8.732
5	2005	72.657	24.438	27.028	34.906	0.000	4.978	8.145
5	2006	71.543	23.133	34.961	35.733	0.000	4.973	8.164
5	2007	72.423	23.087	27.282	37.863	0.000	5.113	8.091
5	2008	68.973	19.651	32.227	39.629	0.000	5.125	8.064
4	1999	11.585	4.442	11.415	6.145	0.000	1.422	0.424
4	2000	11.465	4.153	13.132	5.502	0.000	1.486	0.384
4	2001	11.946	4.302	12.655	5.686	0.000	1.446	0.419
4	2002	11.639	4.262	13.260	6.024	0.000	1.581	0.337
4	2003	13.827	4.040	13.752	5.319	0.000	1.515	0.402
4	2004	13.541	4.372	8.649	5.472	0.000	1.583	0.504
4	2005	13.050	4.496	7.981	6.112	0.000	1.601	0.432
4	2006	13.508	4.480	2.258	7.031	0.000	1.704	0.343
4	2007	13.202	4.884	0.986	6.375	0.000	1.744	0.540
4	2008	14.501	4.571	1.081	6.445	0.000	1.886	0.458
US	1999	374.706	142.074	97.968	226.399	28.123	32.709	20.722
US	2000	379.240	142.348	98.874	233.902	29.030	32.829	22.894
US	2001	375.561	140.570	91.942	215.304	35.380	34.187	25.299
US	2002	370.806	140.287	82.816	212.953	28.123	34.721	26.830
US	2003	391.451	142.841	92.817	199.261	37.195	34.017	27.705
US	2004	393.037	144.125	92.594	191.134	33.566	36.394	29.278
US	2005	378.765	142.535	84.724	193.381	37.195	36.594	28.844
US	2006	396.448	143.871	100.591	197.536	30.844	39.353	32.100
US	2007	392.867	139.933	58.889	189.152	35.380	41.829	44.916
US	2008	377.056	130.069	61.051	201.191	39.009	42.682	44.801
Energy factor <sup>c</sup>		39.82 GJ/m <sup>3</sup>	39.98 GJ/m <sup>3</sup>	38.66 GJ/m <sup>3</sup>	38.27 MJ/m <sup>3</sup>	25.80 MJ/kg	3.6 MJ/kWh	2.18 MJ/kg
CO <sub>2</sub> emission factor (kg/GJ) <sup>c</sup>		67.73	107.74	73.20	55.98	99.58	187.78	91.63

# Supporting Information

**Table S1 continued**

US Refinery product yields <sup>a</sup> --										
District	Year	LPG	Fin. motor	Aviation	Kerosine	Kerosine	Distillate	Residual	Naphtha for	
PADD		(%)	gasoline (%)	gasoline (%)	jet fuel (%)	(%)	fuel oil (%)	fuel oil (%)	chem FS (%)	
1	1999	2.5	46.6	0.2	7.0	0.8	26.3	6.5		0.8
1	2000	2.8	45.2	0.2	6.3	0.8	27.9	6.8		0.8
1	2001	2.9	45.8	0.2	5.3	0.8	29.1	6.6		0.8
1	2002	3.0	46.7	0.3	5.3	0.8	28.1	5.7		0.9
1	2003	3.0	46.4	0.2	5.2	0.8	27.2	7.8		0.8
1	2004	2.6	46.5	0.4	6.1	0.7	26.6	6.9		0.8
1	2005	2.4	46.6	0.3	5.7	0.7	28.8	6.2		0.8
1	2006	2.6	45.8		5.1	0.4	29.2	7.1		1.1
1	2007	3.2	45.5	0.1	5.0	0.5	29.4	7.2		1.1
1	2008	3.3	44.6		5.7	0.6	29.6	7.1		1.1
2	1999	3.7	51.1	0.1	6.6	0.5	24.8	1.6		0.6
2	2000	3.7	50.4	0.1	6.9	0.4	25.7	1.8		0.5
2	2001	3.6	51.1	0.1	6.6	0.4	26.0	2.0		0.6
2	2002	3.5	52.0	0.1	6.7	0.3	25.4	1.8		0.6
2	2003	3.3	51.5	0.1	6.2	0.3	26.0	1.7		0.5
2	2004	3.3	51.6	0.1	6.4	0.3	25.7	1.8		0.8
2	2005	3.1	50.4	0.1	6.5	0.3	27.1	1.6		0.8
2	2006	4.0	49.4	0.1	6.2	0.3	27.3	1.7		0.9
2	2007	3.9	49.8	0.1	6.1	0.1	28.2	1.7		0.9
2	2008	3.5	48.5	0.1	6.3	0.0	30.0	1.6		0.8
3	1999	6.1	44.8	0.2	11.1	0.4	21.1	4.3		2.1
3	2000	6.0	44.7	0.1	11.1	0.4	21.9	4.6		2.2
3	2001	5.6	44.3	0.1	10.5	0.6	22.8	4.8		1.7
3	2002	5.8	45.4	0.1	10.3	0.4	22.3	3.7		2.7
3	2003	5.5	44.8	0.1	9.9	0.4	23.0	4.1		2.6
3	2004	5.3	44.6	0.1	10.0	0.5	23.5	3.9		2.8
3	2005	4.7	43.8	0.1	10.2	0.6	24.5	3.9		2.3
3	2006	4.8	43.5	0.2	9.7	0.4	25.2	3.8		1.9
3	2007	5.0	43.2	0.1	9.4	0.3	26.0	4.1		1.9
3	2008	5.1	41.6	0.1	9.6	0.0	28.4	4.0		1.5
5	1999	2.6	44.7	0.1	15.8	0.2	18.3	8.5		0.2
5	2000	3.1	45.7	0.1	16.2	0.2	18.5	6.8		0.1
5	2001	2.7	45.5	0.1	16.0	0.1	19.2	6.9		0.1
5	2002	2.7	47.3	0.1	16.0	0.1	19.0	6.2		0.1
5	2003	2.9	47.2	0.1	16.0	0.0	19.5	5.8		0.1
5	2004	2.6	47.3	0.1	16.2	0.0	19.5	6.1		0.0
5	2005	2.5	47.3	0.1	16.2	0.0	20.4	5.8		0.0
5	2006	2.8	47.7	0.1	15.3	0.0	20.3	5.8		0.0
5	2007	2.8	46.6	0.1	15.6	0.0	20.8	6.3		0.0
5	2008	2.8	45.6	0.1	17.5	0.0	21.6	5.5		0.0
4	1999	1.3	47.8	0.1	5.4	0.5	28.7	2.3		
4	2000	1.3	47.1	0.1	5.8	0.3	29.1	2.0		0.0
4	2001	1.3	47.4	0.1	5.3	0.3	29.8	2.3		
4	2002	1.1	48.0	0.1	4.8	0.4	29.9	2.1		
4	2003	0.8	47.9	0.1	4.9	0.4	29.5	2.4		
4	2004	0.8	47.5	0.1	4.9	0.3	30.4	2.5		
4	2005	0.7	46.0	0.1	5.4	0.3	30.6	2.7		
4	2006	1.3	46.4	0.1	5.3	0.4	30.6	2.8		
4	2007	1.5	46.3	0.1	5.4	0.3	29.8	2.6		
4	2008	1.6	47.4	0.1	4.8	0.2	31.6	2.2		
US	1999	4.5	46.5	0.2	10.2	0.4	22.3	4.6		1.3
US	2000	4.5	46.2	0.1	10.3	0.4	23.1	4.5		1.3
US	2001	4.3	46.2	0.1	9.8	0.5	23.8	4.6		1.1
US	2002	4.3	47.3	0.1	9.8	0.4	23.2	3.9		1.6
US	2003	4.2	46.9	0.1	9.5	0.4	23.7	4.2		1.5
US	2004	4.0	46.8	0.1	9.7	0.4	23.9	4.1		1.6
US	2005	3.6	46.2	0.1	9.8	0.4	25.0	4.0		1.4
US	2006	3.9	45.8	0.1	9.3	0.3	25.4	4.0		1.2
US	2007	4.1	45.5	0.1	9.1	0.2	26.1	4.2		1.3
US	2008	4.1	44.2	0.1	9.7	0.1	27.8	4.0		1.0
Energy factor <sup>c</sup>		--	--	--	--	--	--	--	--	--
CO <sub>2</sub> emission		--	--	--	--	--	--	--	--	--
factor (kg/GJ) <sup>c</sup>		--	--	--	--	--	--	--	--	--



# Supporting Information

**Table S1 continued**

US		Refinery product yields <sup>a</sup>							Utilization of		
District	Year	Oth. oils for	Special	Lubricants	Waxes	Petroleum	Asphalt &	Fuel gas	Miscellaneous	operable ref.	
PADD		chem FS (%)	naphtha (%)	(%)	(%)	coke (%)	road oil (%)	(%)	products (%)	capacity <sup>a</sup> (%)	
1	1999		0.1	1.0	0.0	3.1	5.4	3.7	0.1	90.9	
1	2000		0.1	0.9	0.1	3.0	6.1	3.5	0.1	91.7	
1	2001		0.1	0.9	0.0	3.3	6.0	3.8	0.1	87.2	
1	2002		0.1	1.0	0.0	3.1	6.0	3.9	0.1	88.9	
1	2003		0.1	1.0	0.0	2.9	5.7	3.8	0.1	92.7	
1	2004		0.1	1.1	0.0	3.1	6.2	3.9	0.1	90.4	
1	2005		0.1	1.0	0.0	2.9	5.7	3.8	0.1	93.1	
1	2006		0.1	1.1	0.0	3.0	5.6	3.6	0.2	86.7	
1	2007		0.0	1.0	0.0	3.2	5.0	3.9	0.2	85.6	
1	2008		0.0	1.1	0.1	3.3	5.1	3.8	0.2	80.8	
2	1999	0.7	0.7	0.6	0.1	4.2	5.6	3.9	0.3	93.3	
2	2000	0.4	0.7	0.5	0.1	4.3	5.5	3.9	0.3	94.2	
2	2001	0.0	0.6	0.4	0.1	4.3	5.1	4.0	0.3	93.9	
2	2002	0.0	0.5	0.5	0.1	4.1	5.3	4.0	0.4	90.0	
2	2003	0.0	0.6	0.5	0.1	4.2	5.6	4.1	0.4	91.6	
2	2004	0.3	0.1	0.4	0.1	4.3	5.7	4.1	0.4	93.6	
2	2005	0.3	0.2	0.4	0.1	4.5	5.7	4.1	0.5	92.9	
2	2006	0.2	0.2	0.5	0.1	4.4	6.1	4.1	0.5	92.4	
2	2007	0.2	0.1	0.4	0.1	4.3	5.3	4.2	0.4	90.1	
2	2008	0.2	0.1	0.4	0.1	4.3	5.3	4.0	0.4	88.4	
3	1999	2.5	0.8	1.7	0.2	4.8	1.7	4.1	0.4	94.7	
3	2000	2.3	0.4	1.7	0.2	4.8	1.8	4.1	0.4	93.9	
3	2001	2.1	0.4	1.6	0.1	5.3	1.6	4.1	0.5	94.8	
3	2002	1.9	0.4	1.6	0.1	5.7	1.6	4.2	0.5	91.5	
3	2003	2.3	0.4	1.5	0.1	5.7	1.6	4.4	0.5	93.6	
3	2004	2.4	0.5	1.6	0.1	5.9	1.5	4.3	0.4	94.1	
3	2005	2.1	0.4	1.6	0.1	6.0	1.6	4.3	0.4	88.3	
3	2006	2.4	0.4	1.7	0.1	6.2	1.5	4.6	0.5	88.7	
3	2007	2.4	0.5	1.7	0.1	6.0	1.3	4.3	0.5	88.7	
3	2008	2.3	0.5	1.7	0.1	6.0	1.1	4.4	0.6	83.6	
5	1999	0.3	0.1	1.0	0.0	6.1	2.4	5.8	0.2	87.1	
5	2000	0.3	0.1	0.9	-0.1	6.3	2.4	5.6	0.3	87.5	
5	2001	0.3	0.1	1.0	0.0	6.0	2.1	5.8	0.3	89.1	
5	2002	0.3	0.1	0.8	0.0	6.0	2.1	5.5	0.3	90.0	
5	2003	0.3	0.1	0.8		6.2	1.9	5.6	0.3	91.3	
5	2004	0.3	0.0	0.7		6.1	1.9	5.4	0.3	90.4	
5	2005	0.4	0.0	0.7		6.2	1.7	5.1	0.3	91.7	
5	2006	0.4	0.1	0.7		6.0	1.8	5.2	0.4	90.5	
5	2007	0.3	0.0	0.6		5.8	1.8	5.4	0.4	87.6	
5	2008	0.1	0.0	0.8		6.1	1.4	5.1	0.5	88.1	
4	1999	0.1	0.0		0.7	3.4	8.8	4.1	0.4	95.7	
4	2000	0.1	0.0		0.6	3.3	9.3	3.9	0.4	94.7	
4	2001	0.2	0.0		0.6	3.3	8.6	4.1	0.4	90.7	
4	2002	0.1			0.5	3.2	9.2	3.8	0.4	91.6	
4	2003	0.1			0.4	3.2	9.1	4.5	0.4	91.9	
4	2004	0.1			0.4	3.2	9.3	4.2	0.4	95.7	
4	2005	0.1	0.0		0.4	3.3	9.5	4.1	0.4	95.5	
4	2006	0.1	0.0		0.3	3.3	8.5	4.2	0.4	93.5	
4	2007	0.1	0.0		0.0	3.4	8.9	4.2	0.3	91.3	
4	2008		0.0		0.0	4.6	6.1	4.6	0.5	89.4	
US	1999	1.4	0.6	1.2	0.1	4.7	3.3	4.3	0.3	92.6	
US	2000	1.3	0.4	1.2	0.1	4.7	3.4	4.2	0.4	92.6	
US	2001	1.1	0.3	1.1	0.1	4.9	3.1	4.3	0.4	92.6	
US	2002	1.0	0.3	1.1	0.1	5.1	3.2	4.3	0.4	90.7	
US	2003	1.2	0.3	1.1	0.1	5.1	3.2	4.5	0.4	92.6	
US	2004	1.3	0.3	1.1	0.1	5.2	3.2	4.4	0.4	93.0	
US	2005	1.1	0.2	1.1	0.1	5.3	3.2	4.3	0.4	90.6	
US	2006	1.2	0.2	1.2	0.1	5.3	3.2	4.5	0.4	89.7	
US	2007	1.3	0.3	1.1	0.1	5.2	2.9	4.4	0.4	88.5	
US	2008	1.2	0.3	1.1	0.1	5.3	2.7	4.3	0.5	85.3	
Energy factor <sup>c</sup>		--	--	--	--	--	--	--	--	--	
CO <sub>2</sub> emission		--	--	--	--	--	--	--	--	--	
factor (kg/GJ) <sup>c</sup>											

## Supporting Information

**Table S1 continued**

US													
Energy consumed/volume crude feed (GJ/m <sup>3</sup> ) and CO <sub>2</sub> emitted/vol. crude feed (kg/m <sup>3</sup> ) for refinery fuels <sup>c</sup>													
District	Year	Hydrogen prod.		Crude oil consmd.		LPG consumed		Distillate consmd.		Res. fuel oil cons.		Fuel gas (bl)	
PADD		(GJ/m <sup>3</sup> )	(kg/m <sup>3</sup> )	(GJ/m <sup>3</sup> )	(kg/m <sup>3</sup> )	(GJ/m <sup>3</sup> )	(kg/m <sup>3</sup> )	(GJ/m <sup>3</sup> )	(kg/m <sup>3</sup> )	(GJ/m <sup>3</sup> )	(kg/m <sup>3</sup> )	(GJ/m <sup>3</sup> )	(kg/m <sup>3</sup> )
1	1999	0.195	10.28	0.000	0.00	0.008	0.52	0.009	0.68	0.173	14.39	1.446	97.93
1	2000	0.230	12.10	0.000	0.00	0.014	0.93	0.018	1.38	0.180	14.94	1.410	95.49
1	2001	0.199	10.48	0.000	0.00	0.017	1.14	0.040	3.11	0.217	18.03	1.498	101.43
1	2002	0.171	8.99	0.000	0.00	0.013	0.85	0.033	2.57	0.138	11.44	1.529	103.58
1	2003	0.242	12.77	0.000	0.00	0.022	1.44	0.042	3.22	0.127	10.57	1.530	103.66
1	2004	0.244	12.88	0.000	0.00	0.022	1.46	0.031	2.43	0.082	6.86	1.548	104.85
1	2005	0.243	12.82	0.000	0.00	0.032	2.08	0.024	1.87	0.082	6.81	1.523	103.13
1	2006	0.297	15.66	0.000	0.00	0.016	1.02	0.002	0.13	0.071	5.88	1.559	105.58
1	2007	0.230	12.13	0.000	0.00	0.009	0.58	0.002	0.12	0.064	5.33	1.695	114.82
1	2008	0.244	12.85	0.000	0.00	0.003	0.17	0.002	0.17	0.033	2.73	1.673	113.30
2	1999	0.334	17.58	0.000	0.00	0.036	2.33	0.002	0.15	0.093	7.71	1.560	105.64
2	2000	0.328	17.31	0.000	0.00	0.019	1.23	0.001	0.12	0.072	5.99	1.556	105.41
2	2001	0.367	19.34	0.000	0.00	0.019	1.23	0.003	0.20	0.084	7.02	1.590	107.72
2	2002	0.347	18.30	0.000	0.00	0.023	1.48	0.002	0.17	0.066	5.53	1.563	105.85
2	2003	0.320	16.89	0.000	0.00	0.035	2.32	0.001	0.09	0.021	1.74	1.553	105.19
2	2004	0.316	16.66	0.000	0.00	0.023	1.51	0.001	0.09	0.007	0.56	1.647	111.58
2	2005	0.381	20.07	0.000	0.00	0.016	1.09	0.002	0.12	0.006	0.47	1.653	111.96
2	2006	0.592	31.19	0.000	0.00	0.012	0.79	0.001	0.11	0.007	0.59	1.635	110.72
2	2007	0.612	32.26	0.000	0.00	0.018	1.20	0.002	0.12	0.007	0.55	1.665	112.80
2	2008	0.616	32.46	0.000	0.00	0.017	1.14	0.001	0.11	0.007	0.57	1.644	111.34
3	1999	0.530	27.94	0.000	0.01	0.008	0.52	0.002	0.14	0.000	0.02	1.771	119.92
3	2000	0.533	28.06	0.000	0.00	0.008	0.53	0.003	0.20	0.000	0.00	1.778	120.40
3	2001	0.545	28.70	0.000	0.00	0.007	0.44	0.002	0.15	0.000	0.00	1.676	113.50
3	2002	0.576	30.33	0.000	0.00	0.008	0.55	0.001	0.10	0.000	0.00	1.753	118.71
3	2003	0.559	29.49	0.000	0.00	0.011	0.70	0.001	0.05	0.000	0.00	1.833	124.18
3	2004	0.592	31.19	0.000	0.00	0.003	0.23	0.001	0.09	0.000	0.00	1.748	118.37
3	2005	0.609	32.08	0.000	0.00	0.003	0.23	0.001	0.10	0.000	0.01	1.693	114.67
3	2006	0.560	29.49	0.000	0.00	0.003	0.17	0.002	0.12	0.000	0.00	1.850	125.28
3	2007	0.553	29.12	0.000	0.00	0.002	0.13	0.002	0.13	0.000	0.00	1.782	120.72
3	2008	0.594	31.28	0.000	0.00	0.005	0.34	0.002	0.12	0.000	0.00	1.774	120.17
5	1999	1.217	64.13	0.000	0.00	0.031	2.05	0.010	0.80	0.025	2.04	1.892	128.17
5	2000	1.426	75.15	0.000	0.00	0.056	3.66	0.009	0.71	0.029	2.44	1.881	127.39
5	2001	1.364	71.86	0.000	0.00	0.075	4.93	0.011	0.82	0.035	2.92	1.899	128.59
5	2002	1.363	71.85	0.000	0.00	0.031	2.02	0.008	0.60	0.037	3.04	1.722	116.63
5	2003	1.315	69.32	0.000	0.00	0.053	3.49	0.009	0.70	0.029	2.41	1.776	120.32
5	2004	1.315	69.29	0.000	0.00	0.038	2.50	0.009	0.66	0.029	2.40	1.774	120.15
5	2005	1.312	69.15	0.000	0.00	0.055	3.65	0.009	0.71	0.029	2.38	1.720	116.48
5	2006	1.409	74.24	0.000	0.00	0.036	2.36	0.009	0.73	0.031	2.55	1.708	115.69
5	2007	1.484	78.18	0.000	0.00	0.036	2.34	0.009	0.69	0.030	2.53	1.781	120.60
5	2008	1.471	77.54	0.000	0.00	0.038	2.48	0.011	0.85	0.030	2.52	1.682	113.92
4	1999	0.448	23.59	0.000	0.00	0.006	0.37	0.001	0.10	0.049	4.08	1.574	106.62
4	2000	0.446	23.50	0.000	0.00	0.008	0.50	0.001	0.05	0.067	5.58	1.534	103.86
4	2001	0.481	25.36	0.000	0.00	0.005	0.35	0.001	0.11	0.049	4.10	1.614	109.29
4	2002	0.465	24.49	0.000	0.00	0.006	0.39	0.000	0.00	0.045	3.70	1.518	102.84
4	2003	0.441	23.22	0.000	0.00	0.006	0.43	0.000	0.00	0.036	3.01	1.787	121.02
4	2004	0.434	22.88	0.000	0.00	0.008	0.56	0.000	0.01	0.030	2.51	1.668	112.99
4	2005	0.631	33.28	0.000	0.00	0.003	0.20	0.000	0.00	0.034	2.82	1.593	107.92
4	2006	0.637	33.58	0.000	0.00	0.002	0.12	0.000	0.00	0.025	2.06	1.664	112.71
4	2007	0.847	44.66	0.000	0.00	0.002	0.11	0.000	0.00	0.017	1.44	1.659	112.38
4	2008	0.983	51.82	0.000	0.00	0.006	0.42	0.000	0.00	0.010	0.86	1.843	124.81
US	1999	0.570	30.01	0.000	0.01	0.018	1.19	0.004	0.31	0.044	3.69	1.705	115.48
US	2000	0.612	32.23	0.000	0.00	0.020	1.28	0.005	0.39	0.042	3.48	1.701	115.21
US	2001	0.619	32.64	0.000	0.00	0.023	1.49	0.007	0.57	0.047	3.92	1.679	113.70
US	2002	0.629	33.14	0.000	0.00	0.016	1.05	0.006	0.45	0.036	3.01	1.676	113.53
US	2003	0.613	32.32	0.000	0.00	0.025	1.62	0.006	0.50	0.024	1.99	1.732	117.31
US	2004	0.625	32.94	0.000	0.00	0.016	1.04	0.005	0.42	0.016	1.32	1.709	115.74
US	2005	0.654	34.49	0.000	0.00	0.019	1.24	0.005	0.40	0.016	1.35	1.668	113.00
US	2006	0.701	36.92	0.000	0.00	0.012	0.79	0.003	0.23	0.015	1.23	1.744	118.10
US	2007	0.713	37.57	0.000	0.00	0.012	0.80	0.003	0.22	0.014	1.13	1.745	118.18
US	2008	0.744	39.23	0.000	0.00	0.014	0.90	0.003	0.26	0.011	0.88	1.722	116.62
Energy factor <sup>c</sup>		16.4 MJ/m <sup>3</sup>		38.49 GJ/m <sup>3</sup>		25.62 GJ/m <sup>3</sup>		38.66 GJ/m <sup>3</sup>		41.72 GJ/m <sup>3</sup>		39.82 GJ/m <sup>3</sup>	
CO <sub>2</sub> emission		--	52.70	--	78.53	--	65.76	--	77.18	--	83.14	--	67.73
factor (kg/GJ) <sup>c</sup>													

## Supporting Information

**Table S1 continued**

US District	Year	Energy consumed/volume crude feed (GJ/m <sup>3</sup> ) and CO <sub>2</sub> emitted/vol. crude feed (kg/m <sup>3</sup> ) for refinery fuels <sup>c</sup>											
PADD		Petroleum coke	Other products	Natural gas	Coal consumed	Electricity purch.	Steam purch.						
		(GJ/m <sup>3</sup> )	(kg/m <sup>3</sup> )	(GJ/m <sup>3</sup> )	(kg/m <sup>3</sup> )	(GJ/m <sup>3</sup> )	(kg/m <sup>3</sup> )	(GJ/m <sup>3</sup> )	(kg/m <sup>3</sup> )	(GJ/m <sup>3</sup> )	(kg/m <sup>3</sup> )	(GJ/m <sup>3</sup> )	(kg/m <sup>3</sup> )
1	1999	0.921	99.186	0.030	2.21	0.493	27.63	0.008	0.81	0.128	24.10	0.039	3.58
1	2000	0.845	91.022	0.026	1.91	0.532	29.76	0.008	0.77	0.123	23.07	0.046	4.19
1	2001	0.883	95.103	0.024	1.78	0.442	24.72	0.009	0.87	0.145	27.14	0.046	4.18
1	2002	0.850	91.531	0.026	1.87	0.479	26.84	0.008	0.82	0.134	25.07	0.046	4.21
1	2003	0.855	92.078	0.030	2.17	0.334	18.72	0.008	0.81	0.134	25.11	0.040	3.64
1	2004	0.894	96.342	0.010	0.70	0.386	21.58	0.007	0.74	0.135	25.30	0.056	5.16
1	2005	0.878	94.557	0.009	0.68	0.416	23.28	0.008	0.83	0.137	25.64	0.052	4.80
1	2006	0.813	87.620	0.004	0.28	0.455	25.48	0.008	0.84	0.149	28.03	0.066	6.01
1	2007	0.890	95.924	0.002	0.11	0.364	20.37	0.009	0.87	0.168	31.51	0.067	6.13
1	2008	0.961	103.488	0.002	0.16	0.374	20.95	0.009	0.90	0.187	35.11	0.064	5.84
2	1999	0.607	65.353	0.045	3.26	0.515	28.80	0.000	0.00	0.165	30.93	0.014	1.29
2	2000	0.593	63.855	0.037	2.72	0.581	32.52	0.000	0.02	0.163	30.57	0.010	0.90
2	2001	0.576	62.009	0.041	3.00	0.528	29.58	0.001	0.08	0.164	30.73	0.023	2.14
2	2002	0.593	63.869	0.040	2.96	0.558	31.24	0.000	0.00	0.172	32.34	0.028	2.53
2	2003	0.585	62.985	0.034	2.48	0.547	30.60	0.001	0.11	0.171	32.10	0.030	2.75
2	2004	0.529	56.979	0.056	4.11	0.584	32.72	0.001	0.10	0.178	33.48	0.033	2.99
2	2005	0.573	61.755	0.054	3.94	0.600	33.59	0.001	0.10	0.185	34.71	0.026	2.37
2	2006	0.546	58.853	0.063	4.59	0.647	36.24	0.000	0.04	0.197	36.92	0.038	3.44
2	2007	0.531	57.224	0.013	0.95	0.692	38.76	0.001	0.09	0.202	37.97	0.057	5.18
2	2008	0.507	54.586	0.001	0.04	0.800	44.76	0.001	0.15	0.207	38.80	0.058	5.30
3	1999	0.649	69.972	0.030	2.16	1.386	77.61	0.000	0.00	0.122	22.82	0.048	4.39
3	2000	0.654	70.430	0.032	2.36	1.369	76.62	0.000	0.00	0.127	23.76	0.061	5.55
3	2001	0.633	68.217	0.028	2.07	1.255	70.23	0.000	0.00	0.135	25.42	0.068	6.22
3	2002	0.650	69.991	0.020	1.48	1.207	67.59	0.000	0.00	0.141	26.51	0.078	7.12
3	2003	0.642	69.143	0.027	2.00	1.100	61.57	0.000	0.00	0.133	25.04	0.074	6.82
3	2004	0.640	68.933	0.020	1.47	0.985	55.12	0.000	0.00	0.141	26.49	0.074	6.81
3	2005	0.628	67.654	0.019	1.40	1.026	57.46	0.000	0.00	0.143	26.88	0.082	7.53
3	2006	0.677	72.950	0.028	2.07	1.002	56.08	0.000	0.00	0.157	29.40	0.090	8.26
3	2007	0.633	68.154	0.022	1.58	0.916	51.27	0.000	0.00	0.171	32.16	0.146	13.39
3	2008	0.613	66.029	0.026	1.87	1.011	56.60	0.000	0.00	0.182	34.23	0.154	14.15
5	1999	0.553	59.534	0.065	4.78	0.868	48.60	0.000	0.00	0.127	23.78	0.121	11.04
5	2000	0.567	61.118	0.064	4.71	0.931	52.13	0.000	0.00	0.110	20.67	0.115	10.50
5	2001	0.565	60.863	0.054	3.95	0.826	46.24	0.000	0.00	0.105	19.65	0.106	9.74
5	2002	0.554	59.655	0.054	3.92	0.907	50.76	0.000	0.00	0.105	19.77	0.101	9.27
5	2003	0.571	61.570	0.060	4.37	0.861	48.17	0.000	0.00	0.098	18.33	0.112	10.30
5	2004	0.589	63.411	0.073	5.34	0.814	45.60	0.000	0.00	0.106	19.83	0.115	10.51
5	2005	0.581	62.572	0.062	4.55	0.794	44.45	0.000	0.00	0.107	20.00	0.106	9.67
5	2006	0.555	59.745	0.081	5.93	0.820	45.90	0.000	0.00	0.107	20.16	0.107	9.78
5	2007	0.570	61.399	0.065	4.77	0.895	50.08	0.000	0.00	0.114	21.34	0.109	9.98
5	2008	0.481	51.835	0.076	5.58	0.929	51.99	0.000	0.00	0.113	21.22	0.108	9.86
4	1999	0.606	65.292	0.151	11.02	0.802	44.92	0.000	0.00	0.175	32.80	0.032	2.89
4	2000	0.558	60.087	0.171	12.48	0.707	39.60	0.000	0.00	0.180	33.74	0.028	2.57
4	2001	0.583	62.862	0.166	12.15	0.738	41.32	0.000	0.00	0.177	33.16	0.031	2.84
4	2002	0.558	60.150	0.168	12.29	0.755	42.28	0.000	0.00	0.186	35.01	0.024	2.21
4	2003	0.524	56.473	0.173	12.63	0.661	36.98	0.000	0.00	0.177	33.24	0.028	2.61
4	2004	0.541	58.265	0.103	7.57	0.648	36.27	0.000	0.00	0.176	33.11	0.034	3.12
4	2005	0.551	59.384	0.095	6.93	0.717	40.15	0.000	0.00	0.177	33.19	0.029	2.64
4	2006	0.554	59.705	0.027	1.98	0.832	46.60	0.000	0.00	0.190	35.64	0.023	2.12
4	2007	0.616	66.398	0.012	0.88	0.770	43.10	0.000	0.00	0.198	37.21	0.037	3.41
4	2008	0.583	62.831	0.013	0.98	0.787	44.07	0.000	0.00	0.217	40.69	0.032	2.92
US	1999	0.649	69.932	0.043	3.17	0.990	55.43	0.001	0.08	0.135	25.27	0.052	4.73
US	2000	0.641	69.064	0.043	3.15	1.008	56.44	0.001	0.08	0.133	25.00	0.056	5.15
US	2001	0.631	67.966	0.040	2.92	0.925	51.78	0.001	0.10	0.138	25.94	0.062	5.67
US	2002	0.637	68.598	0.036	2.66	0.925	51.79	0.001	0.08	0.142	26.65	0.066	6.08
US	2003	0.635	68.369	0.040	2.92	0.847	47.44	0.001	0.11	0.136	25.55	0.067	6.15
US	2004	0.629	67.782	0.039	2.86	0.799	44.71	0.001	0.09	0.143	26.86	0.070	6.39
US	2005	0.630	67.916	0.036	2.65	0.819	45.83	0.001	0.11	0.146	27.36	0.070	6.37
US	2006	0.635	68.447	0.043	3.14	0.835	46.74	0.001	0.09	0.156	29.38	0.077	7.08
US	2007	0.624	67.229	0.025	1.86	0.807	45.20	0.001	0.10	0.168	31.54	0.109	10.01
US	2008	0.596	64.249	0.027	1.98	0.883	49.43	0.001	0.11	0.176	33.09	0.112	10.26
Energy factor <sup>c</sup>		39.98 GJ/m <sup>3</sup>		38.66 GJ/m <sup>3</sup>		38.27 MJ/m <sup>3</sup>		25.80 MJ/kg		3.60 MJ/kWh		2.18 MJ/kg	
CO <sub>2</sub> emission		--	107.74	--	73.20	--	55.98	--	99.58	--	187.78	--	91.63
factor (kg/GJ) <sup>c</sup>													

## Supporting Information

**Table S1 continued**

US		Refinery energy	Fuel mix emission	Refinery carbon
District	Year	consumed ( $EI$ ) <sup>d</sup>	intensity ( $CO_2$ ) <sup>d</sup>	dioxide emissions <sup>d</sup>
PADD		(GJ/m <sup>3</sup> )	(kg/GJ)	(kg/m <sup>3</sup> )
1	1999	3.451	81.53	281.3
1	2000	3.430	80.34	275.6
1	2001	3.518	81.85	288.0
1	2002	3.426	81.08	277.8
1	2003	3.364	81.51	274.2
1	2004	3.416	81.46	278.3
1	2005	3.404	81.23	276.5
1	2006	3.440	80.40	276.5
1	2007	3.499	82.28	287.9
1	2008	3.551	83.26	295.7
2	1999	3.368	78.10	263.1
2	2000	3.361	77.56	260.6
2	2001	3.396	77.46	263.1
2	2002	3.393	77.90	264.3
2	2003	3.298	78.00	257.3
2	2004	3.376	77.25	260.8
2	2005	3.496	77.27	270.2
2	2006	3.738	75.84	283.5
2	2007	3.800	75.55	287.1
2	2008	3.858	74.97	289.3
3	1999	4.546	71.61	325.5
3	2000	4.563	71.87	327.9
3	2001	4.348	72.43	315.0
3	2002	4.434	72.71	322.4
3	2003	4.381	72.81	319.0
3	2004	4.204	73.43	308.7
3	2005	4.205	73.24	308.0
3	2006	4.367	74.15	323.8
3	2007	4.226	74.93	316.7
3	2008	4.361	74.48	324.8
5	1999	4.908	70.27	344.9
5	2000	5.189	69.09	358.5
5	2001	5.039	69.38	349.6
5	2002	4.881	69.15	337.5
5	2003	4.885	69.40	339.0
5	2004	4.861	69.89	339.7
5	2005	4.774	69.88	333.6
5	2006	4.862	69.32	337.1
5	2007	5.091	69.12	351.9
5	2008	4.939	68.39	337.8
4	1999	3.843	75.90	291.7
4	2000	3.698	76.25	282.0
4	2001	3.846	75.80	291.6
4	2002	3.726	76.06	283.4
4	2003	3.833	75.56	289.6
4	2004	3.644	76.10	277.3
4	2005	3.830	74.80	286.5
4	2006	3.955	74.48	294.5
4	2007	4.159	74.43	309.6
4	2008	4.475	73.61	329.4
US	1999	4.211	73.46	309.3
US	2000	4.261	73.09	311.5
US	2001	4.172	73.51	306.7
US	2002	4.170	73.62	307.0
US	2003	4.126	73.74	304.3
US	2004	4.052	74.08	300.2
US	2005	4.065	73.98	300.7
US	2006	4.222	73.94	312.1
US	2007	4.221	74.34	313.8
US	2008	4.289	73.90	317.0
Energy factor <sup>c</sup>		--	--	--
CO <sub>2</sub> emission		--	--	--
factor (kg/GJ) <sup>c</sup>				



**Legend and notes for Table S1.**

Observations of operating refineries that support the central analysis reported in the main text are based on the data given in Table S1.

- a. Refinery crude inputs, fuels consumed, products yield, and capacity utilization are from the U.S. Energy Information Administration (USEIA) (*S1-6*). Fuel energy consumption for hydrogen production is discussed below. Blank entries for yield of some minor products in some districts and years were blank in the original data reported (*S5*) and were assigned a value of zero in the analysis.
- b. Process capacities are volumes that can be processed during 24 hours after making allowances for types and grades of inputs and products, environmental constraints and scheduled downtime, from *Oil & Gas Journal* (*S7*). The prefix “cs” or “ps” denotes processing of crude streams (including gas oil and residua) or of product streams, respectively (csHydrotreating thus includes hydrotreating of gas oil, residua and catalytic cracking feeds). Atmospheric and vacuum distillation capacities reported for the BP Ferndale, WA, and Carson, CA, refineries in 2007 are higher than those in 2006 or 2008 although no distillation upgrades are reported at those plants in 2006 or 2007, and reported vacuum distillation capacity exceeded total crude capacity reported at the Ferndale plant (*S7*). The reported data for those four entries are replaced by the average of 2006 and 2008 atmospheric, and vacuum distillation, capacities for each of those two plants. This results in  $49.609 \cdot 10^4$  instead of  $50.047 \cdot 10^4$  m<sup>3</sup>/day for atmospheric distillation, and  $24.031 \cdot 10^4$  instead of  $26.709 \cdot 10^4$  m<sup>3</sup>/day for vacuum distillation, in those District 5 entries shown for 2007. Analyses including the reported data, including the corrected data, and excluding the observation (for District 5 in 2007), showed that this correction did not affect the results

significantly.

- c. Contributions of refinery fuels to refinery energy consumption/m<sup>3</sup> crude feed (GJ/m<sup>3</sup>) and refinery mass emissions of CO<sub>2</sub> (kg/m<sup>3</sup> crude feed) are shown. These contributions are calculated using the fuel consumption reported and the energy and emission factors shown below each fuel in the table. The energy factor for hydrogen is for an efficient natural gas-fueled steam methane reforming unit as discussed below. Steam energy is based on latent heat of evaporation at 153 kPa/126 °C. All other factors for conversions to common energy units (HHV) are from the California Air Resources Board (*S8*). Emission factors (except for H<sub>2</sub> production) are the fuel emission factors for CO<sub>2</sub> emission from stationary combustion established by USEIA for its voluntary reporting of greenhouse gases program (*S9*). These emission factors are based on carbon content and oxidation estimates for U.S. fuels quality that the agency derived and documented for its estimates of greenhouse gas emissions in the U.S. (*S10*). The U.S. grid average factor is applied to purchased electricity. The average of distillate, LPG, and waste oil blended with distillate fuel factors is applied to the “other products” category.

Energy consumed by hydrogen production cannot be calculated from the USEIA fuels data (*S11*, *S12*). However, the strong trend of hydroprocessing and hydrogen plant capacity addition shown in Table S1 suggests that U.S. refineries were generally hydrogen-limited, and used most of their available H<sub>2</sub> capacity, during 1999-2008. Energy requirements are assigned to 90% of the hydrogen production capacity reported (*S7*) for these reasons. Energy use for steam reforming of natural gas ranges by approximately 15-18 MJ/m<sup>3</sup> H<sub>2</sub> produced (*S12-15*), and is greater for less efficient designs and for plants using heavier feeds such as

naphtha. The energy factor used here ( $16.4 \text{ MJ/m}^3$ ) is for a modern steam methane reformer using pressure swing absorption and natural gas feed (*S13*). The  $\text{CO}_2$  emissions factor ( $52.7 \text{ kg/GJ}$ ) is derived from the same source (*S13*) and is virtually identical to USEPA's estimate of  $0.053 \text{ t/MM Btu}$  (*S15*). Steam reformer  $\text{CO}_2$  emissions are primarily from the shift reaction rather than direct combustion, and increase with the use of heavier feeds and less efficient hydrogen production methods (*S12*, *S15*). Because many refinery hydrogen plants use less efficient technology, naphtha feed or both, the factors used are conservative.

- d. Refinery energy intensity (*EI*) ( $\text{GJ/m}^3$  crude feed), fuel mix emission intensity ( $\text{kg/GJ}$ ), and emissions ( $\text{kg/m}^3$ ) are shown in the last three columns of the table. *EI* ranges by 57%, from  $3.30$  to  $5.19 \text{ GJ/m}^3$  crude feed, while fuel mix emission intensity ranges from  $68.4$  to  $83.3 \text{ kg/GJ}$  (22%) among districts and years. The much larger percentage range for *EI* indicates that differences in total amounts of fuel energy used per volume crude processed have a greater impact on total emissions than differences in the emission intensity of the fuel mix, for these districts and years.

Fuel gas, natural gas, petroleum coke and hydrogen (assumed to be natural gas-fueled herein) account for the vast majority of energy and emissions in all cases but the fuel mix varies between districts and years. Fuel gas accounts for 34% of total energy and emissions in District 5 during 2008, but it accounts for 49% of total energy and 43% of total emissions in District 2 during 2004. Natural gas excluding  $\text{H}_2$  production accounts for 10% of energy and 7% of emissions in District 1 during 2003 but 30% of energy and 24% of emissions in District 3 during 1999. Hydrogen accounts for 5% of energy and 3% of emissions in District 1 during 2002, but 30% of energy and 23% of emissions in District 5 during 2008.

## Supporting Information

Petroleum coke accounts for 10% of energy and 15% of emissions in District 5 during 2008, but it accounts for 27% of energy and 35% of emissions in District 1 during both 1999 and 2008.

Fuel mix emission intensity generally increases with the portion of fuel mix emissions accounted for by coke, which increases with the catalytic cracking/ atmospheric distillation ratio, among districts and years. Petroleum coke is a byproduct of cracking reactions that is burned in cracking catalyst regeneration. Catalytic cracking generally decreases with increasing hydrocracking (capacities/atm. capacity). At the same time, hydrogen production capacity increases with hydrocracking capacity, and with crude feed density. (Other variables also relate to crude density and sulfur content as described in the main text.) Although it varies much less than *EI*, fuel mix emission intensity decreases as *EI*, crude feed density, and crude feed sulfur content increase, among these districts and years.



# Supporting Information

**Table S2. Simplified mixing analysis for potential effects of anomalous oils on crude feeds.**

PADD Year	Refinery crude feed volume data reported <sup>a</sup>				Anomalous oil assumption <sup>c</sup>		Potential crude feed effect <sup>d</sup>	
	Potentially anomalous streams <sup>b</sup> Stream 1 (% vol.)	Stream 2 (% vol.)	Stream 3 (% vol.)	Other streams (% vol.)	Predicted by density, sulfur (factor)	Excess in anomalous oil (factor)	Crude feed predicted (factor)	Crude feed with anomaly (factor)
1 1999	16.59	14.62	10.82	57.97	1	2	1.00	1.27
1 2000	19.73	11.91	11.51	56.85	1	2	1.00	1.29
1 2001	20.49	12.87	11.51	55.13	1	2	1.00	1.30
1 2002	17.28	12.96	12.32	57.44	1	2	1.00	1.27
1 2003	21.93	14.15	13.46	50.46	1	2	1.00	1.32
1 2004	27.74	12.61	11.06	48.59	1	2	1.00	1.37
1 2005	29.46	13.42	11.68	45.44	1	2	1.00	1.39
1 2006	29.89	14.12	12.27	43.72	1	2	1.00	1.40
1 2007	26.88	17.86	11.21	44.05	1	2	1.00	1.39
1 2008	23.23	18.71	10.97	47.09	1	2	1.00	1.35
2 1999	24.01	5.50	4.49	66.00	1	2	1.00	1.28
2 2000	26.90	5.78	4.00	63.32	1	2	1.00	1.31
2 2001	29.08	5.84	3.33	61.75	1	2	1.00	1.33
2 2002	29.40	5.50	1.93	63.17	1	2	1.00	1.33
2 2003	30.82	5.57	2.52	61.09	1	2	1.00	1.34
2 2004	32.02	4.66	2.26	61.06	1	2	1.00	1.35
2 2005	31.35	3.99	2.46	62.20	1	2	1.00	1.34
2 2006	34.76	4.83	1.63	58.78	1	2	1.00	1.38
2 2007	34.73	4.97	2.17	58.13	1	2	1.00	1.38
2 2008	36.35	4.52	1.94	57.19	1	2	1.00	1.39
3 1999	16.50	14.22	11.78	57.50	1	2	1.00	1.27
3 2000	16.77	14.99	13.60	54.64	1	2	1.00	1.28
3 2001	17.72	15.26	14.84	52.18	1	2	1.00	1.29
3 2002	19.61	14.82	14.71	50.86	1	2	1.00	1.31
3 2003	20.18	14.82	14.64	50.36	1	2	1.00	1.31
3 2004	20.21	15.55	12.22	52.02	1	2	1.00	1.31
3 2005	20.52	14.40	11.24	53.84	1	2	1.00	1.31
3 2006	20.53	13.07	10.73	55.67	1	2	1.00	1.30
3 2007	18.39	13.28	11.69	56.64	1	2	1.00	1.28
3 2008	16.61	13.08	12.52	57.79	1	2	1.00	1.26
4 1999	29.57	70.13	0.30	0.00	1	2	1.00	1.65
4 2000	33.07	66.93	0.00	0.00	1	2	1.00	1.67
4 2001	38.31	61.69	0.00	0.00	1	2	1.00	1.69
4 2002	43.61	56.39	0.00	0.00	1	2	1.00	1.72
4 2003	47.16	52.84	0.00	0.00	1	2	1.00	1.74
4 2004	46.77	53.23	0.00	0.00	1	2	1.00	1.73
4 2005	48.29	51.71	0.00	0.00	1	2	1.00	1.74
4 2006	49.87	50.13	0.00	0.00	1	2	1.00	1.75
4 2007	50.99	49.01	0.00	0.00	1	2	1.00	1.75
4 2008	49.10	50.90	0.00	0.00	1	2	1.00	1.75
5 1999	31.84	5.02	3.25	59.89	1	2	1.00	1.35
5 2000	33.00	5.21	3.80	57.99	1	2	1.00	1.37
5 2001	31.84	5.44	4.25	58.47	1	2	1.00	1.36
5 2002	30.86	3.89	3.59	61.66	1	2	1.00	1.34
5 2003	27.61	8.74	3.75	59.90	1	2	1.00	1.33
5 2004	26.28	8.95	5.50	59.27	1	2	1.00	1.32
5 2005	25.14	10.90	6.48	57.48	1	2	1.00	1.32
5 2006	24.26	10.05	6.88	58.81	1	2	1.00	1.31
5 2007	24.68	9.16	5.92	60.24	1	2	1.00	1.31
5 2008	24.34	10.23	7.58	57.85	1	2	1.00	1.31

**Legend and notes for Table S2.**

Density and sulfur content can predict unreported characteristics of crude oils more reliably in well-mixed crude feeds than in poorly mixed crude feeds. When multiple streams each comprise a small portion of the feed, if an oil stream of divergent quality is present, it will have less potential to change the quality of the total crude feed. Table S2 presents results from a simplified four-component mixing analysis for potential effects of anomalous oils on the crude feeds processed in each district and year. These results indicate that the District 4 crude feed is less well mixed than those of other districts.

- a. Refinery crude feed component streams, shown in percent of total crude feed volume for simplicity of presentation, are from USEIA data on gross crude oil inputs to atmospheric distillation and refinery crude oil imports (*S1*, *S3*), and California Energy Commission data on refinery inputs of crude produced in California (*S16*).
- b. Potentially anomalous streams might be dominated by oils in which unreported characteristics that affect processing occur in anomalously high amounts. The three streams with highest potential to effect the crude feed in this way are shown for each district and year. Component streams of crude feeds are ranked based on their potential for anomalous oil and their volume. Oils from the Western Canadian Sedimentary Basin (WCSB) dominate the highest-ranked stream (stream 1) for districts 2 and 4. The WCSB oil stream includes substantial heavy oil and bitumen sources, which tend to be high in nitrogen and vanadium (*S17-19*), and some of this stream is partially pre-processed (*Table S3*). The other streams are ranked based on their volume and the assumption that oils from a single country of origin or U.S. region may originate from similar geology and have similar anomalies. This

## Supporting Information

assumption is made to assess the reliability of predictions based on density and sulfur for these crude feeds where more complete data for specific crude feeds are not available, and may overstate the potential for anomalies in the crude feeds processed by districts 1, 2, 3 and 5. The origins (*S3*, *S16*) and ranks of streams are as follows.

District 1 streams are ranked by volume for country of origin, with Nigeria supplying the largest volume (stream 1) in all years. Stream 2 was from Canada, Angola or Saudi Arabia, stream 3 was from Saudi Arabia, Venezuela, Angola or Norway, and 17-21 countries supplied other streams processed in District 1 annually. District 2 processed Canadian crude as its largest import (stream 1) each year, and its other streams are ranked by volume for foreign country of origin. Stream 2 was from Saudi Arabia in all years, stream 3 was from Nigeria, Venezuela or Algeria, and 12-20 countries supplied other streams refined in District 2 annually. District 3 streams are ranked by volume for foreign country of origin, and Mexico supplied the largest of these inputs (stream 1) in all years. Streams 2 and 3 were from Saudi Arabia or Venezuela, and 25-38 countries supplied other streams refined in District 3 annually.

District 4 processed Canadian crude as its largest import stream in all years, with virtually all of the balance from the U.S., and little or none of its crude feed came from any other country. The Canadian stream (stream 1) is dominated by oils from the WCSB, which have known potential for anomalies. Specific origins of the equal or larger U.S. stream are not reported, however, parts of the WCSB and other oil deposits with similar geology are located in District 4 (*S17*). Limiting crude transport logistics in the landlocked Rocky Mountain states, which are unique to District 4 and help to explain the limited scope of its

imports relative to those of other districts, might also result in reliance on locally produced U.S. feeds. This circumstantial evidence suggests, but does not confirm, the possibility that both the imported and domestic oils refined here might have similar anomalies. Because of this possibility the U.S. stream refined in District 4 is ranked second (stream 2).

District 5 processes substantial amounts of crude from California and Alaska. The California stream (stream 1) is larger than that from any single foreign country, and includes oils from the San Joaquin Valley, which tend to have high density relative to their sulfur content (*Table S9*). The other streams are ranked by volume for foreign country of origin. Stream 2 was from Iraq or Saudi Arabia, stream 3 was from Ecuador, Iraq or Saudi Arabia, and 20-27 countries supplied other crude oil streams refined in District 5 annually.

- c. An unreported characteristic that affects processing is assumed twice as abundant in the anomalous oil as predicted by the density and sulfur content of that oil. The assumed factor of two appears plausible based on the variability observed for nitrogen, vanadium and nickel in whole crude oils. For example, among all assays of crude oils by NETL after 1969 where density, sulfur, nitrogen and residua yield are reported ( $N = 728$ ) (*S20*), the highest-divergent 1% of oils had 1.85 times as much nitrogen by weight as predicted by density and sulfur (nonparametric regression by LOWESS,  $R^2 = 0.71$ ). Real anomalies could vary from this factor, but since it is applied to all districts and years, results will scale in proportion to the factor chosen. A lower or higher factor would thus decrease or increase values for all results, but would not change the results for any differences between districts and years. The predicted and (assumed) excess abundance of the unreported characteristic are shown, for the anomalous oil, in the columns under note (c).

## Supporting Information

- d. These results estimate, for each district and year, the potential for crude feeds to have anomalous high content for unreported characteristics that are not predicted by crude feed density and sulfur. They do not show that any such anomaly actually occurred. Potential effects in the total refinery crude feed assume that the anomalous oil is 100% of stream 1, 50% of stream 2, and 25% of stream 3 for each district and year. The percentages are discounted sequentially because of the decreasing likelihood of the same anomaly in multiple separate streams. The predicted factor is assigned to the balance of the streams for each district and year. Results are shown as increases from the predicted crude feed factor of 1.00 on the right of the table.

Relatively well-mixed crude feeds limit the effect of the anomaly in districts 1, 2, 3 and 5 to less than half of its assumed magnitude in the anomalous oil stream. This compares with crude sulfur concentrations four to eight times those of nitrogen and 160 to 500 times those of nickel and vanadium (*S17*). The ranges of annual estimates for these districts overlap, or adjoin for districts 3 and 5. However, the estimates for District 4 are significantly larger (range: 1.65-1.75) than those for the other districts (combined range: 1.26-1.40). Further, although estimates for the other districts represent an extreme case, the assumption that anomalous oil is 50% of stream 2 might understate the potential effects on the District 4 crude feed, in the event that its Canadian and U.S. inputs both have the same anomaly.

This estimate is limited by the simplified four-component blending analysis and anomalous oil stream assumptions described above, and although it shows that unpredicted anomalies are possible in the District 4 crude feed, it represents an extreme and unlikely scenario for districts 1, 2, 3 and 5.

## Supporting Information

**Table S3. Estimate calculation for Canadian synthetic crude oil (SCO) exports to districts and years.**

NR = Not reported

	units	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008
SCO yield from bitumen upgraders											
NEB Canada estimate <sup>a</sup>	(m <sup>3</sup> •10 <sup>6</sup> )	18.8	18.3	20.0	25.2	29.0	34.3	31.0	37.7	39.5	37.9
ERCB Alberta estimate <sup>b</sup>	(m <sup>3</sup> •10 <sup>6</sup> )	18.8	18.6	20.3	25.6	29.5	34.7	31.7	38.2	39.9	37.9
Upgrading method <sup>a,b</sup>											
Hydrocracking-based	(m <sup>3</sup> •10 <sup>6</sup> )	3.2	3.0	3.3	3.4	9.3	11.4	12.7	11.9	12.7	11.7
Coking-based	(m <sup>3</sup> •10 <sup>6</sup> )	15.6	15.6	16.9	22.1	21.9	23.3	19.0	26.3	27.1	26.2
SCO to Canadian refineries <sup>c</sup>											
All Canadian refining	(m <sup>3</sup> •10 <sup>6</sup> )	13.3	12.5	12.9	12.7	12.1	16.0	14.8	15.6	17.2	17.0
Alberta refineries	(m <sup>3</sup> •10 <sup>6</sup> )	10.1	9.9	10.4	9.6	8.6	11.8	11.8	12.3	13.8	13.0
Other refineries	(m <sup>3</sup> •10 <sup>6</sup> )	3.2	2.6	2.5	3.1	3.4	4.2	3.1	3.3	3.4	3.9
SCO removals from Alberta <sup>b</sup>	(m <sup>3</sup> •10 <sup>6</sup> )	8.8	7.4	8.9	14.2	17.4	21.1	18.9	24.1	25.0	25.0
Supply-demand balance											
Yield (NEB)-all refining	(m <sup>3</sup> •10 <sup>6</sup> )	5.5	5.8	7.1	12.5	16.9	18.3	16.2	22.0	22.3	20.9
Removals-other ref.	(m <sup>3</sup> •10 <sup>6</sup> )	5.6	4.8	6.4	11.1	14.0	16.9	15.8	20.8	21.6	21.1
Excess supply estimate	(m <sup>3</sup> •10 <sup>6</sup> )	5.6	5.8	7.1	12.5	16.9	18.3	16.2	22.0	22.3	21.1
Total SCO exports											
Estimated by NEB <sup>d</sup>	(m <sup>3</sup> •10 <sup>6</sup> )	6.5	NR	NR	9.4	NR	NR	17.5	NR	NR	19.5
SCO exports to U.S.											
Estimated by NEB <sup>d</sup>	(m <sup>3</sup> •10 <sup>6</sup> )	6.5	NR	NR	9.4	NR	NR	17.4	NR	NR	19.3
% of total exports	(%)	100.0			100.0			99.3			99.2
Estimated by interpolation with recent supply/export ratio <sup>e</sup>											
	(m <sup>3</sup> •10 <sup>6</sup> )	--	5.9	6.3	--	14.5	17.7	--	22.5	21.7	--
Consolidated estimate	(m <sup>3</sup> •10 <sup>6</sup> )	6.5	5.9	6.3	9.4	14.5	17.7	17.4	22.5	21.7	19.3
Supply-export balance	(m <sup>3</sup> •10 <sup>6</sup> )	-0.9	-0.1	0.8	3.2	2.4	0.6	-1.3	-0.5	0.7	1.8
SCO exports to U.S. refining districts estimated by NEB <sup>d</sup>											
PADD 1	(m <sup>3</sup> •10 <sup>6</sup> )	0.37	NR	NR	0.26	NR	NR	0.77	NR	NR	0.46
PADD 2	(m <sup>3</sup> •10 <sup>6</sup> )	5.36	NR	NR	6.02	NR	NR	11.89	NR	NR	13.68
PADD 3	(m <sup>3</sup> •10 <sup>6</sup> )	0.00	NR	NR	0.27	NR	NR	0.07	NR	NR	0.09
PADD 4	(m <sup>3</sup> •10 <sup>6</sup> )	0.77	NR	NR	2.36	NR	NR	3.25	NR	NR	2.49
PADD 5	(m <sup>3</sup> •10 <sup>6</sup> )	0.00	NR	NR	0.45	NR	NR	1.44	NR	NR	2.62
SCO exports to districts estimated by interpolation with to recent U.S. SCO portions <sup>e</sup>											
PADD 1	(m <sup>3</sup> •10 <sup>6</sup> )	--	0.28	0.24	--	0.49	0.69	--	0.84	0.66	--
PADD 2	(m <sup>3</sup> •10 <sup>6</sup> )	--	4.52	4.41	--	9.53	11.86	--	15.56	15.15	--
PADD 3	(m <sup>3</sup> •10 <sup>6</sup> )	--	0.06	0.12	--	0.30	0.22	--	0.10	0.10	--
PADD 4	(m <sup>3</sup> •10 <sup>6</sup> )	--	0.97	1.30	--	3.35	3.70	--	3.77	3.21	--
PADD 5	(m <sup>3</sup> •10 <sup>6</sup> )	--	0.10	0.20	--	0.87	1.26	--	2.26	2.55	--
U.S. exports-PADDs balance	(m <sup>3</sup> •10 <sup>6</sup> )	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

**Legend and notes for Table S3.**

Table S3 shows data, reported exports, and calculated estimates for synthetic crude oil (SCO) volume exported from Canada and processed in each district and year. Reported SCO exports are estimates, and these are reported as annual volumes at three-year intervals. Values for the years 2000, 2001, 2003, 2004, 2006 and 2007 are estimated by interpolation based on reported data for the two proximate years. For example, reported data for 1999 and 2002 are used to estimate exported SCO processed in 2000. These estimates thus assume there was no unknown factor that changed the relationship of exports to supply or refinery capacity greatly between the estimated year and the years immediately before and after that year. Results indicate differences between districts in SCO inputs, increasing SCO inputs with time for districts 2 and 4, and that, especially in the earlier years, the SCO came mainly from coking-based upgraders. However, the exact volume and refining characteristics of SCO processed in specific districts and years is uncertain. Notes cited in the table further discuss the sources, data quality, and methods for estimates below.

- a. The first estimate of annual SCO yield for 1999-2008 is from the National Energy Board of Canada (NEB) (*S21*).
- b. The second estimate of SCO yield for 1999-2008, and yield by upgrading method for 2000-2008, are from the Energy Resources Conservation Board of Alberta (ERCB) (*S22*). Yield by upgrader in 1999 is from the NEB (*S21*). The exact volumes from coking- and hydrocracking-based upgrading are uncertain. One major upgrader that primarily uses the coking method also uses hydrocracking (*S22*). Most (75%) of the SCO yield from this upgrader is assigned to coking and 25% is assigned to hydrocracking in the table.

## Supporting Information

- c. SCO inputs to Canadian refineries are from Statistics Canada (*S23*). The agency reports these inputs for light SCO, however, some intermediate and heavy crude streams from the Western Canadian Sedimentary Basin (WCSB) are delivered as blends that may contain SCO. The SCO in such blends may not be reported, for some exports or refinery inputs.
- d. SCO exports, including exports to the U.S. and to each U.S. district, are estimated by the NEB for 1999 (*S24*), 2002 (*S25*), 2005 (*S26*), and 2008 (*S27*). The U.S. receives nearly all these exports, however, estimated exports do not balance exactly with the excess supply of SCO estimated to be available after Canadian usage of these oils. NEB export estimates appear to exceed available supply by 0.9 and 1.3 million m<sup>3</sup> in 1999 and 2005, while supply appears to exceed NEB export estimates by 3.2 and 1.8 million m<sup>3</sup> in 2002 and 2008, respectively. This is shown in the “supply-export balance” line of the table. These differences are small for some estimation purposes, but they approach or exceed the total exports estimated for some districts and years. Refining characteristics of the SCO exports are not reported.
- e. Although reported only at three-year intervals, exports increase steadily with supply, and their apportionment among the districts changes little over these intervals. This is explained by the need for disposition of the SCO created, and the unique logistical constraints posed by transport and refining of SCO from the WCSB in each district. These constraints allow a rough estimate of the relative SCO volumes exported and refined in the intervening years.

First, total U.S. exports are estimated for years when they are not reported. The excess supply estimate for each such year is multiplied by the weighted average fraction of supply exported in the two nearest reported years. This weighted average is calculated using a 2:1 ratio to give twice as much weight to the proximate year (e.g., 1999 for the 2000 estimate)



and half as much weight to the year more distant in time (2002 in this example). The supply-export balance line of the table shows that these interpolated estimates generally compare more closely with excess supply than do the reported estimates.

SCO exports to districts are then estimated by apportioning the estimated total U.S. exports for the year to be estimated based on the weighted average of each district's share of total SCO exports in the two nearest reported years. This weighted average is calculated using a 2:1 ratio to give twice as much weight to the proximate year (e.g., 1999 for the 2000 estimate) and half as much weight to the year more distant in time (2002 in this example). The bottom line of the table shows that these SCO estimates for districts balance with total estimated SCO exports to the U.S. for each year.

These estimates should be interpreted with caution as discussed above. Nevertheless, they provide evidence that SCO comprised an appreciable portion of crude refined during some years in District 2, and especially District 4, which refines much less oil in total than other districts (*Table S1*). The estimates suggest that SCO accounts for more than 10% of District 4 crude feeds and up to 8% of District 2 feeds, in some years. Reported and estimated Canadian SCO accounted for less than 2% of the crude feeds processed in districts 1, 3 and 5 during 1999-2008.

# Supporting Information

**Table S 4. Evidence for effects of synthetic oil (SCO) on refinery processing during 1999-2008 in District 4.**

PADD	Year	Refinery observations for selected parameters <sup>a</sup>					SCO % vol. of refinery crude feed <sup>b</sup> (%)	Predictions based on non-SCO feeds <sup>c</sup>				Energy for excess H <sub>2</sub> production/m <sup>3</sup> crude feed <sup>d</sup> (GJ/m <sup>3</sup> ) (% <i>EI</i> )	
		Crude feed density (kg/m <sup>3</sup> )	H <sup>2</sup> prod- uction capacity (m <sup>3</sup> /m <sup>3</sup> )	Conver- sion capacity (m <sup>3</sup> /m <sup>3</sup> )	Crude st- ream hyd- rotreating capacity (m <sup>3</sup> /m <sup>3</sup> )	Refinery energy intensity ( <i>EI</i> ) (GJ/m <sup>3</sup> )		H <sub>2</sub> predicted by crude fd. density		csHydrotreating pred. by conv. cap.			
		Predicted (m <sup>3</sup> /m <sup>3</sup> )	Excess (m <sup>3</sup> /m <sup>3</sup> )	Predicted (m <sup>3</sup> /m <sup>3</sup> )	Excess (m <sup>3</sup> /m <sup>3</sup> )								
1	1999	858.20	13.25	0.516	0.054	3.451	0.41	19.60	--	0.122	--	--	--
1	2000	860.18	15.66	0.525	0.054	3.430	0.31	24.22	--	0.130	--	--	--
1	2001	866.34	12.71	0.481	0.029	3.518	0.28	38.66	--	0.094	--	--	--
1	2002	865.71	11.11	0.474	0.084	3.426	0.30	37.16	--	0.087	--	--	--
1	2003	863.44	16.49	0.474	0.059	3.364	0.53	31.83	--	0.087	--	--	--
1	2004	865.44	16.52	0.475	0.059	3.416	0.76	36.54	--	0.088	--	--	--
1	2005	863.38	16.59	0.476	0.058	3.404	0.83	31.70	--	0.089	--	--	--
1	2006	864.12	18.83	0.476	0.028	3.440	0.98	33.44	--	0.090	--	--	--
1	2007	864.33	14.46	0.476	0.028	3.499	0.77	33.93	--	0.090	--	--	--
1	2008	863.65	14.46	0.476	0.028	3.551	0.57	32.32	--	0.090	--	--	--
2	1999	858.25	21.23	0.486	0.125	3.368	2.74	19.73	1.50	0.097	0.028	0.022	0.66
2	2000	860.03	21.17	0.488	0.107	3.361	2.28	23.85	--	0.099	0.008	--	--
2	2001	861.33	23.18	0.485	0.096	3.396	2.30	26.91	--	0.096	--	--	--
2	2002	861.02	21.58	0.481	0.129	3.393	3.22	26.17	--	0.093	0.035	--	--
2	2003	862.80	20.02	0.477	0.132	3.298	5.09	30.35	--	0.090	0.043	--	--
2	2004	865.65	20.25	0.473	0.148	3.376	6.19	37.04	--	0.087	0.061	--	--
2	2005	865.65	24.07	0.484	0.148	3.496	6.18	37.04	--	0.096	0.052	--	--
2	2006	865.44	37.33	0.488	0.140	3.738	8.10	36.54	0.79	0.099	0.042	0.012	0.31
2	2007	864.07	36.89	0.479	0.137	3.800	8.06	33.31	3.58	0.092	0.045	0.053	1.39
2	2008	862.59	37.12	0.487	0.146	3.858	7.27	29.85	7.26	0.098	0.047	0.107	2.78
3	1999	869.00	32.51	0.566	0.151	4.546	0.00	44.95	--	0.165	--	--	--
3	2000	870.29	33.03	0.579	0.155	4.563	0.01	47.99	--	0.175	--	--	--
3	2001	874.43	34.50	0.600	0.129	4.348	0.03	57.86	--	0.193	--	--	--
3	2002	876.70	34.95	0.611	0.148	4.434	0.07	63.32	--	0.203	--	--	--
3	2003	874.48	34.66	0.604	0.168	4.381	0.07	57.99	--	0.196	--	--	--
3	2004	877.79	37.31	0.610	0.174	4.204	0.05	65.94	--	0.201	--	--	--
3	2005	878.01	35.69	0.588	0.168	4.205	0.02	66.46	--	0.183	--	--	--
3	2006	875.67	33.33	0.587	0.167	4.367	0.02	60.85	--	0.182	--	--	--
3	2007	876.98	32.83	0.594	0.184	4.226	0.02	63.97	--	0.188	--	--	--
3	2008	878.66	33.64	0.600	0.171	4.361	0.02	68.04	--	0.193	--	--	--
4	1999	854.47	28.31	0.415	0.112	3.843	2.64	10.96	17.34	0.040	0.073	0.256	6.66
4	2000	859.35	30.44	0.426	0.092	3.698	3.25	22.27	8.17	0.049	0.043	0.121	3.26
4	2001	859.19	29.92	0.421	0.050	3.846	4.43	21.91	8.01	0.045	0.005	0.118	3.07
4	2002	860.23	29.09	0.404	0.087	3.726	7.73	24.34	4.75	0.031	0.056	0.070	1.88
4	2003	861.23	27.94	0.408	0.087	3.833	10.86	26.66	1.28	0.034	0.053	0.019	0.49
4	2004	862.59	28.02	0.419	0.090	3.644	11.44	29.85	--	0.043	0.047	--	--
4	2005	862.91	41.87	0.407	0.093	3.830	9.98	30.59	11.28	0.034	0.060	0.167	4.35
4	2006	860.50	38.16	0.408	0.109	3.955	11.67	24.95	13.21	0.034	0.075	0.195	4.93
4	2007	862.38	49.76	0.415	0.109	4.159	10.13	29.36	20.39	0.040	0.069	0.301	7.24
4	2008	863.12	59.86	0.409	0.136	4.475	7.94	31.09	28.78	0.035	0.101	0.425	9.49
5	1999	894.61	69.93	0.613	0.195	4.908	0.00	107.06	--	0.204	--	--	--
5	2000	895.85	83.53	0.613	0.167	5.189	0.06	110.15	--	0.204	--	--	--
5	2001	893.76	82.53	0.619	0.174	5.039	0.13	104.95	--	0.209	--	--	--
5	2002	889.99	85.44	0.636	0.196	4.881	0.28	95.65	--	0.224	--	--	--
5	2003	889.10	83.17	0.620	0.165	4.885	0.52	93.45	--	0.210	--	--	--
5	2004	888.87	83.17	0.627	0.167	4.861	0.76	92.90	--	0.216	--	--	--
5	2005	888.99	83.44	0.626	0.166	4.774	0.86	93.18	--	0.216	--	--	--
5	2006	887.65	88.20	0.641	0.160	4.862	1.35	89.89	--	0.228	--	--	--
5	2007	885.54	89.90	0.656	0.167	5.091	1.58	84.73	5.17	0.242	--	0.076	1.50
5	2008	890.16	89.68	0.645	0.163	4.939	1.60	96.07	--	0.232	--	--	--

**Legend and notes for Table S4.**

Table S4 presents results from analysis of synthetic crude oil (SCO) effects on refining.

Canadian export estimates (*Table S3*) suggest that during 1999-2008 SCO from Western Canada was 2-8% and 2-12% of crude feeds in districts 2 and 4, respectively. This SCO stream yields more and lower quality gas oil as compared with typical whole crude oils, and can require more hydroprocessing in refineries (*S24, S25*). Crude density correlates with hydrogen demand for crude oils generally but does not correlate well for some SCO (*S14*). Reported hydrogen capacity is compared with that predicted by crude feed density, and reported crude stream hydrotreating capacity is compared with that predicted by conversion capacity, among districts and years. Crude stream hydrotreating processes gas oil, residua and catalytic cracking feeds (*Table S1*). These comparisons provide information about the relationship of hydrogen production to hydrogen use in processing gas oil, including gas oil from refinery SCO inputs. Hydrogen production in excess of that predicted by crude feed density is then compared with total refinery processing requirements on an energy basis.

Results suggest that SCO affects hydroprocessing and hydrogen production in refineries and may have increased refinery energy intensity significantly during some years in District 4. Hydrogen excesses are found only when SCO was present in crude feeds, and are found during four years in District 2 and nine years in District 4. Hydrotreating excesses are found only when estimated SCO inputs exceeded 2% of crude feeds and occurred during nine years in District 2 and ten years in District 4. The magnitude of hydrogen excesses generally increased with that of hydrotreating excesses and both were larger in District 4 than in District 2. Energy use for excess hydrogen production was minimal in District 2, but in District 4 it exceeded 5% of total

## Supporting Information

refinery energy consumed during three years, and exceeded 9% of total refinery energy in 2008.

The magnitude of hydrogen excesses is not well correlated with the estimated percentage of SCO in crude feeds, especially in District 4. The extent to which this poor correlation reflects unreported changes in the quality of SCO inputs, unreported changes in the quality of the balance of the poorly-mixed District 4 crude feed (*Table S2*), or errors in SCO volume estimates (*Table S3*), could not be determined with available data.

- a. Refinery observations shown on the left of the table are based on the data given in Table S1. Capacities/m<sup>3</sup> atmospheric distillation capacity are shown.
- b. The percentage of total refinery crude feed volume comprised of SCO is estimated based on estimated SCO exports from Table S3 and reported total crude inputs from Table S1. The SCO export estimates are uncertain, as detailed in Table S3.
- c. Predictions shown are from PLS regression on all data for districts where estimated SCO inputs never exceeded 2% of total crude feeds during 1999-2008 (districts 1, 3 and 5). R-squared values are 0.88 for hydrogen production capacity predicted by crude feed density, and 0.85 for crude stream hydrotreating capacity predicted by conversion capacity. These predictions are “blind” to the presence of SCO in that it was not included as a variable in either of these two PLS models. Predictions and excesses shown are based on the upper 95% confidence for observations. Observed values exceed the lower 95% confidence (not shown) for all comparisons.
- d. Energy consumed for the excess in hydrogen production capacity, which is shown as cubic meters H<sub>2</sub>/m<sup>3</sup> atmospheric distillation capacity in this table, is calculated using the energy (16.4 MJ/m<sup>3</sup> H<sub>2</sub>) and capacity utilization (90%) factors from Table S1.

**Table S5. Efficiency factors for processing refinery products.**

Product	Efficiency factor (%)	Average specific gravity
Light liquids		
Gasoline	86.4	0.737
Diesel	91.0	0.845
Kerosine	92.2	0.814
Naphtha	92.7	0.756
Other products		
Lube stocks	80.5	0.889
Waxes	80.5	0.799
Asphalt	84.9	1.038
Coke	86.3	0.967
Fuel gas	90.0	0.844
Heavy fuel oil	91.0	0.946
LPG	92.7	0.539
Residual oil	94.1	0.946

**Legend and notes for Table S5.**

Product-specific processing energy efficiency factors for a current typical U.S. refinery (mass-based) from reference *S11*, and average specific gravities of North American products from reference *S28*. These values were used with yield data from Table S1 to estimate energy use for products processing (“Eproducts”). The Eproducts estimates for refining districts and years are used, with *S*, *d*, capacity utilized, and products ratio observations from data in Table S1, in the Eproducts v. *OQ* comparison reported in Table 1 of the main text.

**Table S6. Estimate calculation, oil quality and processing EI including bitumen upgrading.**

PADD	Year	Refinery observations <sup>a</sup>				Cap. utilized (%)	Prod. ratio (ratio)	Synthetic crude oil input estimate <sup>b</sup>		Coking : hy- drocracking <sup>b</sup> (ratio)
		Crude input (m <sup>3</sup> /d•10 <sup>4</sup> )	Density (kg/m <sup>3</sup> )	S (kg/m <sup>3</sup> )	EI (GJ/m <sup>3</sup> )			(m <sup>3</sup> /d•10 <sup>4</sup> )	(%)	
1	1999	24.436	858.20	8.24	3.451	90.9	3.668	0.101	0.41	4.8
1	2000	24.754	860.18	8.00	3.430	91.7	3.489	0.077	0.31	5.2
1	2001	23.546	866.34	7.71	3.518	87.2	3.479	0.065	0.28	5.2
1	2002	24.246	865.71	7.45	3.426	88.9	3.605	0.073	0.30	6.5
1	2003	25.184	863.44	7.43	3.364	92.7	3.321	0.134	0.53	2.4
1	2004	24.961	865.44	7.79	3.416	90.4	3.398	0.190	0.76	2.0
1	2005	25.422	863.38	7.17	3.404	93.1	3.756	0.212	0.83	1.5
1	2006	23.626	864.12	7.17	3.440	86.7	3.522	0.231	0.98	2.2
1	2007	23.419	864.33	7.26	3.499	85.6	3.443	0.181	0.77	2.1
1	2008	22.115	863.65	7.08	3.551	80.8	3.400	0.125	0.57	2.2
2	1999	53.626	858.25	10.64	3.368	93.3	4.077	1.469	2.74	4.8
2	2000	54.215	860.03	11.35	3.361	94.2	4.132	1.238	2.28	5.2
2	2001	52.609	861.33	11.37	3.396	93.9	4.313	1.210	2.30	5.2
2	2002	51.162	861.02	11.28	3.393	90.0	4.345	1.648	3.22	6.5
2	2003	51.258	862.80	11.65	3.298	91.6	4.281	2.611	5.09	2.4
2	2004	52.482	865.65	11.86	3.376	93.6	4.167	3.250	6.19	2.0
2	2005	52.688	865.65	11.95	3.496	92.9	4.207	3.258	6.18	1.5
2	2006	52.609	865.44	11.60	3.738	92.4	3.907	4.264	8.10	2.2
2	2007	51.480	864.07	11.84	3.800	90.1	4.161	4.152	8.06	2.1
2	2008	51.575	862.59	11.73	3.858	88.4	4.333	3.747	7.27	2.2
3	1999	111.689	869.00	12.86	4.546	94.7	3.120	0.000	0.00	4.8
3	2000	113.024	870.29	12.97	4.563	93.9	3.120	0.015	0.01	5.2
3	2001	115.600	874.43	14.34	4.348	94.8	3.128	0.033	0.03	5.2
3	2002	112.786	876.70	14.47	4.434	91.5	3.251	0.073	0.07	6.5
3	2003	116.013	874.48	14.43	4.381	93.6	3.160	0.081	0.07	2.4
3	2004	119.145	877.79	14.40	4.204	94.1	3.228	0.060	0.05	2.0
3	2005	114.534	878.01	14.40	4.205	88.3	3.316	0.020	0.02	1.5
3	2006	117.253	875.67	14.36	4.367	88.7	3.176	0.027	0.02	2.2
3	2007	117.682	876.98	14.47	4.226	88.7	3.205	0.027	0.02	2.1
3	2008	111.879	878.66	14.94	4.361	83.6	3.229	0.026	0.02	2.2
5	1999	41.973	894.61	11.09	4.908	87.1	2.952	0.001	0.00	4.8
5	2000	43.086	895.85	10.84	5.189	87.5	3.160	0.027	0.06	5.2
5	2001	44.262	893.76	10.99	5.039	89.1	3.231	0.056	0.13	5.2
5	2002	44.787	889.99	10.86	4.881	90.0	3.460	0.124	0.28	6.5
5	2003	45.661	889.10	10.94	4.885	91.3	3.487	0.238	0.52	2.4
5	2004	45.486	888.87	11.20	4.861	90.4	3.551	0.345	0.76	2.0
5	2005	46.090	888.99	11.38	4.774	91.7	3.700	0.394	0.86	1.5
5	2006	45.693	887.65	10.92	4.862	90.5	3.615	0.618	1.35	2.2
5	2007	44.373	885.54	11.07	5.091	87.6	3.551	0.700	1.58	2.1
5	2008	44.739	890.16	12.11	4.939	88.1	3.803	0.717	1.60	2.2
4	1999	8.029	854.47	11.71	3.843	95.1	3.910	0.212	2.64	4.8
4	2000	8.156	859.35	12.03	3.698	94.7	3.943	0.265	3.25	5.2
4	2001	8.077	859.19	11.08	3.846	90.7	3.986	0.357	4.43	5.2
4	2002	8.363	860.23	12.04	3.726	91.6	4.078	0.647	7.73	6.5
4	2003	8.442	861.23	12.49	3.833	91.9	3.962	0.917	10.86	2.4
4	2004	8.856	862.59	11.65	3.644	95.7	3.981	1.013	11.44	2.0
4	2005	8.935	862.91	11.22	3.830	95.5	3.887	0.892	9.98	1.5
4	2006	8.856	860.50	11.36	3.955	93.5	3.962	1.033	11.67	2.2
4	2007	8.681	862.38	11.73	4.159	91.3	3.900	0.879	10.13	2.1
4	2008	8.585	863.12	12.17	4.475	89.4	4.291	0.682	7.94	2.2

# Supporting Information

**Table S6. Estimate calculation, oil quality and processing *EI* including bitumen upgrading.**

*Continued*

PADD	Year	Bitumen upgrading estimate <sup>c</sup>			Upgrading and refining estimate				Estimate compared to OQ prediction <sup>k</sup> (±% 95% Conf.)
		Density <sub>add</sub> <sup>d</sup> (kg/m <sup>3</sup> )	S <sub>add</sub> <sup>e</sup> (kg/m <sup>3</sup> )	EI <sub>add</sub> <sup>f</sup> (GJ/m <sup>3</sup> )	Density <sub>adi</sub> <sup>g</sup> (kg/m <sup>3</sup> )	S <sub>adi</sub> <sup>h</sup> (kg/m <sup>3</sup> )	EI <sub>adi</sub> <sup>i</sup> (GJ/m <sup>3</sup> )	EI <sub>tp</sub> <sup>j</sup> (GJ/m <sup>3</sup> )	
1	1999	0.45	0.17	0.022	858.65	8.41	3.473	3.271	--
1	2000	0.34	0.13	0.017	860.52	8.13	3.447	3.372	--
1	2001	0.30	0.11	0.015	866.65	7.82	3.533	3.579	--
1	2002	0.33	0.12	0.016	866.04	7.57	3.442	3.533	--
1	2003	0.57	0.22	0.030	864.01	7.65	3.394	3.531	--
1	2004	0.81	0.32	0.043	866.25	8.11	3.459	3.623	--
1	2005	0.87	0.35	0.048	864.26	7.52	3.452	3.470	--
1	2006	1.04	0.41	0.055	865.17	7.58	3.495	3.488	--
1	2007	0.82	0.32	0.044	865.16	7.58	3.543	3.489	--
1	2008	0.60	0.24	0.032	864.25	7.32	3.583	3.393	--
2	1999	3.00	1.12	0.148	861.26	11.76	3.516	3.546	--
2	2000	2.51	0.93	0.123	862.53	12.28	3.484	3.634	--
2	2001	2.52	0.94	0.124	863.86	12.31	3.520	3.662	--
2	2002	3.56	1.30	0.172	864.58	12.58	3.565	3.667	--
2	2003	5.45	2.12	0.285	868.25	13.77	3.583	3.925	--
2	2004	6.58	2.59	0.349	872.24	14.45	3.725	4.179	-2%
2	2005	6.48	2.62	0.355	872.14	14.57	3.852	4.168	--
2	2006	8.65	3.39	0.455	874.09	14.98	4.193	4.321	--
2	2007	8.59	3.37	0.454	872.66	15.21	4.254	4.210	--
2	2008	7.75	3.03	0.408	870.35	14.76	4.266	4.038	--
3	1999	0.00	0.00	0.000	869.00	12.86	4.546	4.117	2%
3	2000	0.02	0.01	0.001	870.30	12.97	4.563	4.173	1%
3	2001	0.03	0.01	0.002	874.46	14.35	4.350	4.446	--
3	2002	0.07	0.03	0.004	876.78	14.49	4.437	4.504	--
3	2003	0.07	0.03	0.004	874.56	14.46	4.385	4.440	--
3	2004	0.05	0.02	0.003	877.84	14.42	4.207	4.575	--
3	2005	0.02	0.01	0.001	878.03	14.41	4.206	4.512	--
3	2006	0.02	0.01	0.001	875.70	14.37	4.369	4.434	--
3	2007	0.02	0.01	0.001	877.00	14.48	4.227	4.493	--
3	2008	0.02	0.01	0.001	878.69	14.95	4.362	4.541	--
5	1999	0.00	0.00	0.000	894.61	11.09	4.909	5.082	--
5	2000	0.07	0.03	0.003	895.92	10.87	5.192	5.097	--
5	2001	0.14	0.05	0.007	893.90	11.04	5.046	5.023	--
5	2002	0.31	0.11	0.015	890.30	10.97	4.896	4.834	--
5	2003	0.56	0.22	0.029	889.65	11.15	4.914	4.825	--
5	2004	0.81	0.32	0.043	889.68	11.52	4.903	4.830	--
5	2005	0.90	0.36	0.049	889.88	11.74	4.824	4.841	--
5	2006	1.44	0.57	0.076	889.09	11.48	4.938	4.793	--
5	2007	1.68	0.66	0.089	887.22	11.73	5.180	4.707	2%
5	2008	1.71	0.67	0.090	891.87	12.78	5.029	4.939	--
4	1999	2.89	1.08	0.143	857.36	12.78	3.986	3.482	4%
4	2000	3.57	1.32	0.175	862.91	13.35	3.873	3.750	--
4	2001	4.86	1.80	0.239	864.05	12.88	4.085	3.726	--
4	2002	8.54	3.13	0.414	868.78	15.17	4.139	4.065	--
4	2003	11.62	4.53	0.608	872.85	17.01	4.441	4.377	--
4	2004	12.16	4.79	0.645	874.76	16.44	4.289	4.459	--
4	2005	10.46	4.23	0.574	873.37	15.45	4.404	4.352	--
4	2006	12.45	4.87	0.655	872.94	16.23	4.610	4.349	--
4	2007	10.79	4.24	0.570	873.17	15.96	4.729	4.331	1%
4	2008	8.47	3.31	0.446	871.59	15.48	4.921	4.152	9%

**Legend and notes for Table S6.**

Table S6 presents an estimate of oil quality and processing energy for total oil processing, including refining and pre-processing for that portion of refinery crude feeds comprised of synthetic crude oil (SCO), for each district and year. Coking- and hydrocracking-based bitumen upgrading uses energy to yield SCO of lower density and sulfur content than the bitumen. SCO imported from Western Canada accounts for an estimated 2-8% of total District 2 crude feeds and 2-12% of total District 4 feeds during 1999-2008. Refinery crude feeds and energy consumption do not reflect the original bitumen quality for this SCO or the energy consumed in its upgrading. The estimate shown in this table relates initial oil quality to process energy for total processing. The energy consumed and density and sulfur lost in upgrading is estimated based on process modeling data and added “back” to the refinery crude feed and energy consumption observed. The estimated total process energy is then compared to that predicted by the initial oil quality. Results suggest that in general, total process energy increases with worsening initial oil quality consistent with the prediction based on observed refinery data. The exception involves two results for District 4. This is discussed in note (k).

- a. Refinery feed volume, density, sulfur content (*S*), capacity utilization, and products ratio (calculated as described in the main paper) are from data in Table S1.
- b. Synthetic crude oil (SCO) inputs and sources by upgrader type are from the estimates detailed in Table S3. The volume, percentage of total refinery crude feed volume, and ratio of coking- to hydrocracking-based upgrading for the SCO are shown.
- c. SCO was produced from bitumen in Western Canada by coking-based and hydrocracking-based upgrading (*S22*). Both upgrading schemes typically also use atmospheric and vacuum



distillation and significant hydrotreating, sulfur recovery and hydrogen production. Material and energy inputs and outputs were estimated using process modeling of typical coking-based and hydrocracking-based upgraders yielding SCO from Athabasca bitumen by Keesom et al. (*SI4*). Modeled parameters included, among others, bitumen feed density ( $1.011 \text{ t/m}^3$ ) and sulfur content ( $48.64 \text{ kg/m}^3$ ), SCO yield ( $22,259 \text{ m}^3/\text{d}$ ), and SCO density and sulfur content for the coking-based ( $881.07 \text{ kg/m}^3 \text{ d}$ ,  $3.23 \text{ kg/m}^3 \text{ S}$ ) and hydrocracking-based ( $921.82 \text{ kg/m}^3 \text{ d}$ ,  $3.23 \text{ kg/m}^3 \text{ S}$ ) schemes. Carbon rejection, hydrogen addition and utility energy inputs estimated by process modeling on these parameters were  $4,773 \text{ GJ/h}$  for the coking-based scheme and  $6,155 \text{ GJ/h}$  for the hydrocracking-based scheme (*SI4*). This indicates energy inputs of approximately  $0.04 \text{ GJ}$  per  $\text{kg}$  density (including sulfur) lost from the feed in the SCO from the coking-based scheme, and  $0.07 \text{ GJ/kg}$  for that from the hydrocracking scheme. Energy inputs were not allocated to sulfur removal separately from density reduction in the reported results.

Bitumen feed to the coking- and hydrocracking-based schemes was modeled at 1.15 times and 0.97 times the SCO volume yield, respectively (*SI4*). Thus, on a product volume basis, estimated energy use was approximately  $5.15$  and  $6.64 \text{ GJ per m}^3$  SCO produced for the coking- and hydrocracking-based upgraders, respectively. SCO from the coking- and hydrocracking-based schemes was  $130.22$  and  $89.47 \text{ kg/m}^3$  lighter than the bitumen feed, respectively, and both schemes produced SCO with  $45.41 \text{ kg/m}^3$  less sulfur than the bitumen feed. These estimates are applied to the shares of SCO from coking- and hydrocracking-based upgrading each year to estimate initial oil quality and total process energy. Notes d through f detail the calculations.

## Supporting Information

- d. Density lost in upgrading the bitumen ( $Density_{add}$ ) is added to the total refinery crude feed density to account for the bitumen input processed upstream to produce the SCO.  $Density_{add}$  is calculated as:

$$Density_{add} = SCOvol \cdot (DR \div VC)$$

Where

SCOvol is the percentage of SCO in the total refinery crude feed; DR is the density reduction from bitumen from note (c) in  $kg/m^3$ ; VC is the volume change from bitumen to SCO from note (c); and the result is in  $kg/m^3$  refinery crude feed.

- e. Sulfur lost in upgrading the bitumen ( $S_{add}$ ) is added to the total refinery crude feed sulfur to account for the bitumen input processed upstream to produce the SCO.  $S_{add}$  is calculated as:

$$S_{add} = SCOvol \cdot (45.41 \div VC)$$

Where

SCOvol is the percentage of SCO in the total refinery crude feed; 45.41 is the sulfur content reduction from bitumen from note (c) in  $kg/m^3$ ; VC is the volume change from bitumen to SCO from note (c); and the result is in  $kg/m^3$  refinery crude feed.

- f. Energy lost in upgrading the bitumen ( $EI_{add}$ ) is added to the refinery energy intensity calculated from the data in Table S1 ( $EI$ ) to estimate the total energy intensity of processing the oil feed.  $EI_{add}$  is calculated as:

$$EI_{add} = SCOvol \cdot EC$$

Where

SCOvol is the percentage of SCO in the total refinery crude feed; EC is the energy consumed by upgrading in  $GJ/m^3$  SCO from note (c); and the result is expressed as  $GJ/m^3$  refinery crude feed.

## Supporting Information

- g.  $\text{Density}_{\text{adj}}$  is the sum of crude feed density and  $\text{Density}_{\text{add}}$  and is an estimate of initial crude feed quality accounting for the bitumen feed upgraded to produce SCO refined.
- h.  $S_{\text{adj}}$  is the sum of  $S$  and  $S_{\text{add}}$  and is an estimate of initial crude feed quality accounting for the quality of the bitumen feed upgraded to produce SCO processed in a refinery.
- i.  $EI_{\text{adj}}$  is the sum of  $EI$  and  $EI_{\text{add}}$  and is an estimate of the total energy intensity of processing including upgrading and refining.
- j.  $EI_{\text{tp}}$  is the total *predicted* energy intensity of upgrading and processing and is an estimate of the total energy intensity predicted by the relationship of  $EI$  to crude feed density and sulfur based on the refinery observations.  $EI_{\text{tp}}$  is the result from inputting  $S_{\text{adj}}$ ,  $\text{Density}_{\text{adj}}$ , product ratio and capacity utilized to the prediction mode of the PLS model, which is run on the observations from districts 1, 2, 3 and 5.  $EI_{\text{tp}}$  is compared with  $EI_{\text{adj}}$  in the final column of the table (note k) and in Figure 2.
- k. The final column of the table compares estimated total processing energy ( $EI_{\text{adj}}$ ) with total processing energy predicted by initial oil quality ( $EI_{\text{tp}}$ ). Dashed lines (--) show that the result for estimated energy falls within the 95% confidence of prediction for observations. Negative values (e.g., -1%) show the percentage by which any result falls below the 95% confidence of prediction. Positive values (e.g., 1%) show the percentage by which any result exceeds the 95% confidence of prediction.

Estimated  $EI_{\text{adj}}$  is within the prediction based on oil quality or within 3% of its confidence interval in 48 of 50 cases. The exceptions are excesses for the years 1999 and 2008 in District 4. These excesses can be attributed to high excess hydrogen production in District 4 during those years (*Table S4*). It is possible that those high hydrogen values were

related to increased hydroprocessing needs for SCO, or for some other anomaly, in the District 4 crude feed during those years. The need for hydrogen addition to address the poor gas oil and distillate product qualities of SCO (*S24, S25*) and its variable quality (*S14, S24*) support this possibility. This possibility cannot be confirmed or excluded, because the SCO input volume is uncertain (*Table S3*), its quality is unknown, and there is a potential for other sources of variability in the poorly-mixed District 4 crude feed (*Table S2*).

## Supporting Information

**Table S7.** Contribution of CO<sub>2</sub> to CO<sub>2</sub>e emitted by oil refineries.

	Units	CO <sub>2</sub>	CH <sub>4</sub>	N <sub>2</sub> O
Refinery emissions mass				
Scope				
U.S. (NETL)	Mt/y	257.90	0.1656	0.0040
U.S. (EPA)	Mt/y	228.53	0.0873	0.0007
California	Mt/y	35.54	0.0015	0.0001
Global warming potential				
20-yr. horizon	Factor	1	62	275
100-yr. horizon	Factor	1	23	296
500-yr. horizon	Factor	1	7	156
20-yr. horizon CO <sub>2</sub> e				
U.S. (NETL)	Mt/y	257.90	10.27	1.11
U.S. (EPA)	Mt/y	228.53	5.41	0.19
California	Mt/y	35.54	0.09	0.03
100-yr. horizon CO <sub>2</sub> e				
U.S. (NETL)	Mt/y	257.90	3.81	1.19
U.S. (EPA)	Mt/y	228.53	2.01	0.21
California	Mt/y	35.54	0.03	0.03
500-yr. horizon CO <sub>2</sub> e				
U.S. (NETL)	Mt/y	257.90	1.16	0.63
U.S. (EPA)	Mt/y	228.53	0.61	0.11
California	Mt/y	35.54	0.01	0.02
Range of percent total CO <sub>2</sub> e				
20-yr. horizon	Percent	95.78-99.66	0.26-3.81	0.08-0.41
100-yr. horizon	Percent	98.10-99.82	0.10-1.45	0.08-0.45
500-yr. horizon	Percent	99.31-99.93	0.03-0.45	0.04-0.24

**Legend and notes for Table S7.** (Mt/y, megatons per year.) U.S. refinery emission estimates are reported as mass emitted (NETL) (*S25*) and as CO<sub>2</sub>e emitted (EPA) (*S29*). California refinery emissions are reported as mass emitted (*S30*). Global warming potential is from the Intergovernmental Panel on Climate Change (*S31*). The U.S. (EPA) emissions mass estimate is calculated from reported CO<sub>2</sub>e (*S29*) and 100-year global warming potential (*S31*). The percent of total CO<sub>2</sub>e from CO<sub>2</sub> and the small differences between estimates shown in Table S7 support the finding that CO<sub>2</sub> dominates refinery greenhouse gas emissions.

## Supporting Information

**Table S8. PLS inputs for CO<sub>2</sub> emissions predicted by OQ, and comparison emission estimates.**

(NA, not applicable; value predicted by OQ)

PADD	Year	Density (kg/m <sup>3</sup> )	Sulfur (kg/m <sup>3</sup> )	Cap.	Prod.	Observed	Predicted <i>EI</i> (95% conf.)			Fuel mix
				utilzd. (%)	ratio (ratio)	<i>EI</i> (GJ/m <sup>3</sup> )	Lower (GJ/m <sup>3</sup> )	Central (GJ/m <sup>3</sup> )	Upper (GJ/m <sup>3</sup> )	em. intensity (kg/GJ)
1	1999	858.20	8.24	90.9	3.668	3.451	2.877	3.241	3.604	81.53
1	2000	860.18	8.00	91.7	3.489	3.430	2.987	3.349	3.711	80.34
1	2001	866.34	7.71	87.2	3.479	3.518	3.198	3.559	3.919	81.85
1	2002	865.71	7.45	88.9	3.605	3.426	3.152	3.511	3.870	81.08
1	2003	863.44	7.43	92.7	3.321	3.364	3.133	3.493	3.853	81.51
1	2004	865.44	7.79	90.4	3.398	3.416	3.209	3.568	3.927	81.46
1	2005	863.38	7.17	93.1	3.756	3.404	3.048	3.410	3.772	81.23
1	2006	864.12	7.17	86.7	3.522	3.440	3.054	3.417	3.780	80.40
1	2007	864.33	7.26	85.6	3.443	3.499	3.067	3.433	3.800	82.28
1	2008	863.65	7.08	80.8	3.400	3.551	2.972	3.352	3.733	83.26
2	1999	858.25	10.64	93.3	4.077	3.368	2.984	3.347	3.711	78.11
2	2000	860.03	11.35	94.2	4.132	3.361	3.104	3.468	3.832	77.56
2	2001	861.33	11.37	93.9	4.313	3.396	3.126	3.495	3.863	77.46
2	2002	861.02	11.28	90.0	4.345	3.393	3.068	3.432	3.796	77.90
2	2003	862.80	11.65	91.6	4.281	3.298	3.195	3.558	3.922	78.00
2	2004	865.65	11.86	93.6	4.167	3.376	3.369	3.733	4.098	77.25
2	2005	865.65	11.95	92.9	4.207	3.496	3.362	3.725	4.089	77.27
2	2006	865.44	11.60	92.4	3.907	3.738	3.380	3.738	4.095	75.84
2	2007	864.07	11.84	90.1	4.161	3.800	3.270	3.629	3.989	75.55
2	2008	862.59	11.73	88.4	4.333	3.858	3.154	3.515	3.875	74.97
3	1999	869.00	12.86	94.7	3.120	4.546	3.759	4.117	4.476	71.61
3	2000	870.29	12.97	93.9	3.120	4.563	3.813	4.172	4.531	71.87
3	2001	874.43	14.34	94.8	3.128	4.348	4.085	4.444	4.803	72.43
3	2002	876.70	14.47	91.5	3.251	4.434	4.140	4.499	4.859	72.71
3	2003	874.48	14.43	93.6	3.160	4.381	4.076	4.435	4.794	72.81
3	2004	877.79	14.40	94.1	3.228	4.204	4.213	4.572	4.930	73.43
3	2005	878.01	14.40	88.3	3.316	4.205	4.149	4.511	4.873	73.24
3	2006	875.67	14.36	88.7	3.176	4.367	4.067	4.432	4.798	74.15
3	2007	876.98	14.47	88.7	3.205	4.226	4.127	4.491	4.856	74.93
3	2008	878.66	14.94	83.6	3.229	4.361	4.165	4.540	4.915	74.48
5	1999	894.61	11.09	87.1	2.952	4.908	4.713	5.082	5.451	70.27
5	2000	895.85	10.84	87.5	3.160	5.189	4.725	5.092	5.460	69.09
5	2001	893.76	10.99	89.1	3.231	5.039	4.648	5.014	5.380	69.38
5	2002	889.99	10.86	90.0	3.460	4.881	4.450	4.814	5.178	69.15
5	2003	889.10	10.94	91.3	3.487	4.885	4.422	4.788	5.153	69.40
5	2004	888.87	11.20	90.4	3.551	4.861	4.410	4.775	5.140	69.89
5	2005	888.99	11.38	91.7	3.700	4.774	4.409	4.780	5.151	69.88
5	2006	887.65	10.92	90.5	3.615	4.862	4.331	4.695	5.060	69.32
5	2007	885.54	11.07	87.6	3.551	5.091	4.235	4.594	4.953	69.12
5	2008	890.16	12.11	88.1	3.803	4.939	4.456	4.824	5.191	68.39
<b>Other inputs</b>										
US	2002	873.89	12.32	90.7	3.534	NA	3.838	4.194	4.549	73.62
US	2005	875.08	12.43	90.6	3.597	NA	3.885	4.241	4.597	73.98
US	2006	873.78	12.32	89.7	3.458	NA	3.835	4.191	4.547	73.94
US	2007	873.89	12.50	88.5	3.485	NA	3.833	4.190	4.547	74.34
SFBA	2008	899.66	11.91	90.8	3.469	NA	4.938	5.307	5.676	68.39
Heavy oil		957.40	27.80	90.8	3.469	NA	8.228	8.795	9.363	73.77
Nat. bitumen	1	1033.60	45.50	90.8	3.469	NA	12.266	13.200	14.135	73.77

## Supporting Information

**Table S8. PLS inputs for CO<sub>2</sub> emissions predicted by OQ, and comparison emission estimates, *continued*.**

PADD	Year	Central <i>EI</i> prediction (GJ/m <sup>3</sup> )	Fuel mix em. intensity (kg/GJ)	Observed emissions (kg/m <sup>3</sup> )	Predicted emissions (95% conf.)			Comp- arison (± % CI)
					Lower (kg/m <sup>3</sup> )	Central (kg/m <sup>3</sup> )	Upper (kg/m <sup>3</sup> )	
1	1999	3.241	81.53	281	243	265	287	--
1	2000	3.349	80.34	276	249	270	292	--
1	2001	3.559	81.85	288	257	279	301	--
1	2002	3.511	81.08	278	255	277	299	--
1	2003	3.493	81.51	274	254	276	298	--
1	2004	3.568	81.46	278	258	279	301	--
1	2005	3.410	81.23	277	251	272	294	--
1	2006	3.417	80.40	277	252	273	294	--
1	2007	3.433	82.28	288	251	273	295	--
1	2008	3.352	83.26	296	247	269	292	+1.4%
2	1999	3.347	78.11	263	249	271	292	--
2	2000	3.468	77.56	261	254	276	298	--
2	2001	3.495	77.46	263	256	277	299	--
2	2002	3.432	77.90	264	253	274	296	--
2	2003	3.558	78.00	257	259	280	301	-0.5%
2	2004	3.733	77.25	261	267	288	309	-2.2%
2	2005	3.725	77.27	270	266	288	309	--
2	2006	3.738	75.84	284	267	289	310	--
2	2007	3.629	75.55	287	262	284	306	--
2	2008	3.515	74.97	289	256	279	301	--
3	1999	4.117	71.61	326	285	307	328	--
3	2000	4.172	71.87	328	287	309	331	--
3	2001	4.444	72.43	315	300	321	342	--
3	2002	4.499	72.71	322	302	323	345	--
3	2003	4.435	72.81	319	299	320	342	--
3	2004	4.572	73.43	309	305	326	348	--
3	2005	4.511	73.24	308	302	324	345	--
3	2006	4.432	74.15	324	299	320	341	--
3	2007	4.491	74.93	317	301	322	344	--
3	2008	4.540	74.48	325	303	325	346	--
5	1999	5.082	70.27	345	328	350	372	--
5	2000	5.092	69.09	358	329	351	373	--
5	2001	5.014	69.38	350	325	347	369	--
5	2002	4.814	69.15	338	317	338	360	--
5	2003	4.788	69.40	339	315	337	359	--
5	2004	4.775	69.89	340	315	336	358	--
5	2005	4.780	69.88	334	315	337	358	--
5	2006	4.695	69.32	337	311	333	354	--
5	2007	4.594	69.12	352	307	328	350	+0.5%
5	2008	4.824	68.39	338	317	339	361	--
<b>Other inputs</b>								
US	2002	4.194	73.62	315	288	309	331	--
US	2005	4.241	73.98	285	290	311	333	-1.7%
US	2006	4.191	73.94	277	288	309	330	-3.9%
US	2007	4.190	74.34	280	288	309	330	-2.6%
SFBA	2008	5.307	68.39	360	338	360	383	--

**Legend and notes for Table S8.**

Table S8 shows inputs for emissions predicted by crude feed quality and compares the predictions with observed or estimated emissions. Observed crude feed density and sulfur, capacity utilized and products ratio were compared with observed *EI* among districts and years. Predicted *EI* values are the results from this PLS analysis, and are shown for the central prediction and the 95% confidence of prediction for observations. The central *EI* prediction and the observed fuel mix emission intensity were then compared with observed emissions among districts and years. Predicted emissions are the results from this PLS analysis, and are shown for the central prediction and the 95% confidence of prediction for observations. The observations compared among districts and years are from the data in Table S1. Other inputs shown at the bottom of the table were used in the prediction mode of these PLS models.

For U.S. refineries in 2002, 2005, 2006 and 2007, all data except estimated annual emissions are from Table S1. USEIA estimated that U.S. refineries emitted 277.6 megatons (Mt) of CO<sub>2</sub> in 2002 (*S32*). The National Energy Technology Laboratory estimated that U.S. refineries emitted 257.9 Mt in 2005 (*S12*). USEIA estimated that U.S. refineries emitted 250.7 Mt in 2006 and 251.3 Mt in 2007 (*S33*). U.S. refinery crude feed volumes in 2002, 2005, 2006 and 2007 totaled  $241.3 \cdot 10^4$ ,  $247.7 \cdot 10^4$ ,  $248.0 \cdot 10^4$  and  $245.6 \cdot 10^4$  m<sup>3</sup>/day respectively (*Table S1*).

*OQ* inputs for San Francisco Bay Area (SFBA) refineries in 2008 were estimated as detailed in Table S9. The domestic component of SFBA crude feeds was more limited and better characterized than that of refinery crude feeds statewide, and this allowed a more reliable *OQ* estimate for SFBA refining than that which could be derived from publicly reported data for California refineries statewide. Although it has less capacity than Southern California, the SFBA has greater total crude capacity than other refining centers in District 5 (*S7*). The District 5 fuel



mix during 2008 is used for the SFBA prediction to account for fuel mix differences observed among districts (*Table S1*). SFBA inputs for capacity utilized and products ratio were the US averages for 1999-2008 from Table S1. Third party-certified estimates of emissions from SFBA refineries and adjacent plants supplying them hydrogen, as reported by the California Air Resources Board (*S34*), total 17.18 Mt in 2008. Crude feed volume was estimated as the total crude capacity of SFBA refineries in 2008 ( $13.07 \cdot 10^4 \text{ m}^3/\text{day}$ ) reported by *Oil & Gas Journal* (*S7*). This SFBA emissions estimate ( $360 \text{ kg/m}^3$ ) compares with estimated California emissions of  $354 \text{ kg/m}^3$  based on estimated emissions (36.88 Mt) and crude feed volume ( $28.5 \cdot 10^4 \text{ m}^3/\text{day}$ ) for refineries statewide in 2008 (*S34*, *S35*).

The California Air Resources Board (*S36*, *S37*) reported estimated CO<sub>2</sub> emissions from refining the average crude feed in California, including those from bulk vents and refinery fuels acquisition, of 13.34 g/MJ gasoline (CARBOB) and 11.19 g/MJ diesel (ULSD) for 30.10 GJ/m<sup>3</sup> gasoline and 33.86 GJ/m<sup>3</sup> diesel. The California Energy Commission (*S35*) reported 2008 California refinery crude inputs, gasoline (RBOB, CBOB) yield, and diesel ( $\leq 15$  ppm sulfur) yield of 104.04, 51.11 and  $21.61 \text{ m}^3 \cdot 10^6$  respectively (total gasoline and diesel yield was 61.05 and  $23.06 \text{ m}^3 \cdot 10^6$  respectively). These reports suggest refinery emissions of 197.2 and 78.7 kg/m<sup>3</sup> crude refined for California-grade gasoline and diesel production, respectively.

*OQ* inputs for heavy oil and natural bitumen are the average densities and sulfur contents of heavy oil and natural bitumen reported by the U.S. Geologic Survey (*S17*). Other inputs for heavy oil and natural bitumen assume the 1999-2008 U.S. averages based on the data from Table S1. The 1999-2008 fuel mix assumption may be conservative for future emissions from refining lower quality oil, which tends to create more byproduct gases and petroleum coke that could

## Supporting Information

replace some of the natural gas now burned as fuel. Refinery emissions observations were not available for these oils.

The columns on the right of the table compare predicted and observed emissions. Horizontal lines (—) indicate that the result is within the 95% confidence of prediction. Emissions observed among districts and years vary consistently with those predicted by *OQ*, fall within the 95% confidence of prediction in 36 of 40 cases, and fall within 3% of the confidence of prediction in all cases. Emissions estimated by government agencies fall within the prediction in 2 of 5 cases and fall within 4% of its confidence interval in all cases. The agency estimates differ from each other by 12% to 30% while they differ from the central prediction based on *OQ* by 0.1% to 10%.

**Table S9. Estimate calculation, San Francisco Bay Area crude feed OQ in 2008.**

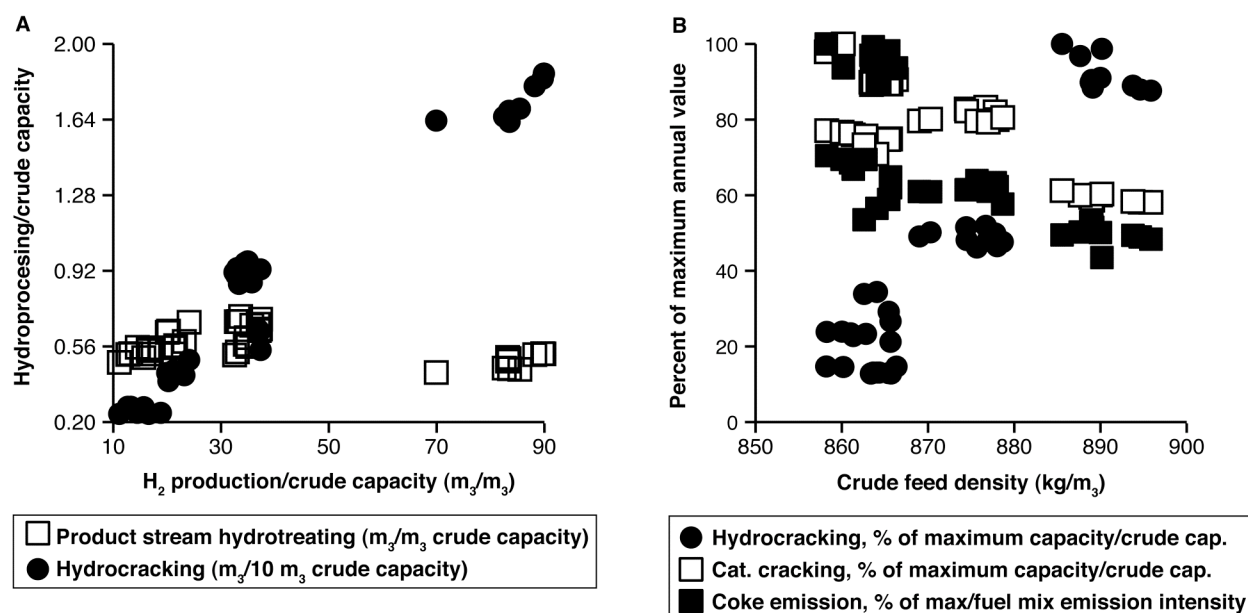
Crude feed vol. (m <sup>3</sup> /d)	Foreign <sup>a</sup>	SJV <sup>b</sup>	ANS <sup>c</sup>	Subtotal <sup>d</sup>
Benicia Plant	8.870•10 <sup>3</sup>	5.323•10 <sup>3</sup>	7.987•10 <sup>3</sup>	2.218•10 <sup>4</sup>
Golden Eagle Plt.	9.683•10 <sup>3</sup>	7.987•10 <sup>3</sup>	7.930•10 <sup>3</sup>	2.560•10 <sup>4</sup>
Martinez Plt.	4.837•10 <sup>3</sup>	1.992•10 <sup>4</sup>	4.592•10 <sup>2</sup>	2.522•10 <sup>4</sup>
Richmond Plt.	2.992•10 <sup>4</sup>	0	8.710•10 <sup>3</sup>	3.863•10 <sup>4</sup>
Rodeo/S. Maria Plt.	1.611•10 <sup>3</sup>	1.450•10 <sup>4</sup>	2.968•10 <sup>3</sup>	1.908•10 <sup>4</sup>
Crude feed mass (kg/d)	Foreign <sup>a</sup>	SJV <sup>e</sup>	ANS <sup>f</sup>	Total
Whole crude	4.827•10 <sup>7</sup>	4.540•10 <sup>7</sup>	2.392•10 <sup>7</sup>	1.176•10 <sup>8</sup>
Sulfur in crude	7.592•10 <sup>5</sup>	5.901•10 <sup>5</sup>	2.076•10 <sup>5</sup>	1.557•10 <sup>6</sup>
		<b>OQ</b>	S (kg/m <sup>3</sup> ) d (kg/m <sup>3</sup> )	<b>11.91</b> <b>899.66</b>

**Legend and notes for Table S9.**

The *OQ* input for the San Francisco Bay Area refineries prediction (*S* and *d*, Table S8) is an estimate based on crude feed from foreign, Alaskan North Slope (ANS) and California oils that assumes transport logistics result in California supply from San Joaquin Valley crude delivered by pipeline (SJV) (*S16*, *S38*). SJV portions of refinery feeds (*S39*) are used with refinery capacities (*S7*) and foreign crude feed volumes (*S40*) to estimate SJV volume processed. ANS volume is then estimated by difference. Weighted average crude feed *OQ* is estimated using these feed volumes and foreign (*S40*), SJV (*S38*, *S41*) and ANS (*S42*) crude quality data.

Superscript notes in Table S9 identify the usage of these data in the estimate calculation specifically:

- Foreign crude feed volume, density and sulfur content reported for each plant (*S40*).
- San Joaquin Valley pipeline crude volume based on SJV percentage of refinery feed reported (*S39*) and crude charge capacities (*S1*).
- Alaskan North Slope (ANS) volume estimated by difference.
- Refinery crude charge capacities from *Oil & Gas Journal* (*S7*).
- Based on SJV volume processed by Bay Area refineries, weighted average density (951.0 kg/m<sup>3</sup>) from available data (*S38*), and sulfur content (12.36 kg/m<sup>3</sup>) (*S41*).
- From ANS volume calculated, and density (860.18 kg/m<sup>3</sup>) and sulfur content (7.40 kg/m<sup>3</sup>) of ANS crude at the Richmond Plant (*S42*).



**Figure S1. Some shifts among hydrogen addition and carbon rejection technologies affecting relationships between (A) hydrotreating and hydrogen production, and (B) fuel mix emission intensity and crude feed density, across refining districts 1, 2, 3 and 5, 1999-2008.** All observations shown are from the data in Table S1.

A. Decreasing hydrotreating/hydrocracking ratio with increasing hydrogen production. Capacities are shown per volume atmospheric crude distillation capacity. Hydrocracking capacities are much smaller than total hydrotreating capacities and are shown at ten-times scale to reveal trends for both types of hydroprocessing. Hydrocracking uses much more hydrogen per volume oil feed than hydrotreating (*S43*), though actual unit  $H_2$  requirements vary by type and quality of feed, unit design, catalyst type and condition, firing rate and quench rate of process units. Hydrocracking increases steadily with hydrogen production while product hydrotreating does not. Hydrotreating increases with  $H_2$  production at lower  $H_2$  production but is lowest at highest  $H_2$  production. Relative to hydrocracking capacity, hydrotreating capacity decreases steadily with increasing  $H_2$  production, from the largest capacity relative to hydrocracking in

## Supporting Information

District 1 ( $\text{H}_2$  capacity 13-19  $\text{m}^3/\text{m}^3$  crude capacity) to the smallest relative to hydrocracking in District 5 ( $\text{H}_2$  capacity 69-90  $\text{m}^3/\text{m}^3$ ).

B. Decreasing petroleum coke contribution to total fuel mix emissions with increasing crude feed density. The portion of total fuel mix emissions accounted for by petroleum coke and the process capacities/volume crude capacity are shown as percentages of the maximum (100%) for each value. The observed increase in hydrocracking with density is consistent with the strong positive associations of hydrogen production with both hydrocracking and density (*Table 1, main text*). Coke accounts for a decreasing portion of fuel mix emissions as crude feed density and hydrocracking increase. This change for coke, which has higher emission intensity than other major refinery fuels, can explain why the fuel mix emission intensity decreases slightly with worsening oil quality (*Table S1*). Despite increasing total conversion capacity (hydrocracking, catalytic cracking, and thermal coking), catalytic cracking capacity per vol. crude capacity decreases as crude feed density and hydrocracking increase. The ratio of catalytic cracking to hydrocracking decreases across districts, following the hydrotreating pattern noted above. Decreasing catalytic cracking explains decreasing coke emissions because cracking catalyst regeneration is a major cause of coke combustion in refineries.

The shifts from hydrotreating and catalytic cracking to hydrocracking observed can explain the coincidence of slightly lower hydrotreating at high hydrogen production, and of slightly decreasing fuel mix emission intensity as crude feed density increases, for these districts and years. Refiners can choose to substitute hydrocracking for hydrotreating and catalytic cracking to some extent, but the relative importance of crude feed quality among the factors that influenced such business decisions is beyond the scope of this study.

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